

FTC	T-O-T	b	omega	T1 label	O label	T2 label	ring-size{ring-number}:Ring Count (unit cell)	average ring size	ring index (this T-site)	BGB energy w.r.t. quartz (eV/TO2)	BS energy w.r.t. quartz (eV/TO2)	Eads (kJ/mol)
JBW	153.2	4.18	26.4	T1	O1	T1	4{1}_6{5}_8{1}	6	4{1}_6{3}	0.07	0.025	116.8
ATN	150.1	4.14	29.8	T1	O2	T1	4{4}_6{8}_8{2}	5.71	6{2}_8{1}	0.08	0.035	116.6
ATT	145.3	4.1	34.7	T1	O4	T1	4{8}_6{2}_8{6}	5.75	4{1}_6{1}_8{2}		0.045	115.2
AFR	141.5	4.05	38.6	T3	O9	T4	4{22}_6{24}_8{4}_12{2}	5.54	4{2}_6{3}	0.126	0.051	115.2
AFO	140.2	4.03	40.3	T3	O7	T3	4{8}_6{84}	5.83	6{8}		0.051	115.1
BEA	138.5	4.01	41.9	T1	O1	T3	4{20}_5{48}_6{8}_12{32}	6.96	4{1}_5{1}_12{3}		0.053	115.1
VFI	125.6	3.81	55.4	T1	O3	T2	4{12}_6{82}	5.74	4{1}_6{6}	0.117	0.054	117.2
MEI	131.2	3.9	49.8	T3	O6	T3	3{2}_4{18}_5{12}_7{6}_12{2}	5.1	3{1}_5{2}	0.129	0.055	115.9
SOS	116.1	3.5	73.9	T3	O6	T3	3{8}_4{8}_6{8}_8{26}_12{2}	6.46	3{2}	0.105	0.059	122.4
-CLO	142.2	4.06	38	T1	O3	T2	4{144}_6{56}_8{9}_12{8}	4.98	4{2}_6{1}		0.059	115.1
EMT	141.4	4.05	38.7	T1	O2	T4	4{72}_6{32}_12{8}	5.14	4{1}_6{1}_12{1}	0.156	0.059	115.1
RWR	135.4	3.96	47.2	T2	O2	T2	4{4}_5{16}_6{24}_8{8}	5.85	4{1}_6{2}_8{1}		0.060	114.0
-RON	138.9	2.52	78.5	T4	O1	T1	4{12}_6{20}_8{16}_10{4}	6.46	6{3}_8{2}	0.113	0.061	184.2
DFT	145.1	4.09	34.9	T1	O1	T1	4{4}_6{8}_8{10}	6.55	4{1}_6{4}_8{5}	0.099	0.064	115.7
SAS	148.1	4.18	31.7	T2	O5	T2	4{20}_6{16}_8{2}	5.05	4{2}_6{1}		0.064	112.3
GOO	124.7	3.8	57.8	T1	O2	T3	4{20}_6{16}_8{32}_10{24}	7.3	4{2}_6{2}_8{1}_10{3}		0.065	115.8
JST	128	3.84	54.8	T1	O1	T1	3{32}_6{4}_10{24}	6	3{1}_6{1}_10{1}		0.066	115.7
MTN	177	4.26	2	T1	O1	T2	5{144}_6{16}	5.1	5{3}	0.111	0.066	131.9
SSF	144.2	4.09	35.9	T1	O4	T1	4{18}_5{12}_6{49}_12{12}	6.26	4{1}_6{2}_12{2}		0.067	114.8
ITW	144	4.08	36.3	T2	O6	T3	4{12}_5{8}_6{4}_8{8}	5.5	4{2}_6{1}	0.124	0.068	115.1
OFF	143.1	4.07	37.1	T1	O2	T1	4{12}_6{6}_8{3}	5.14	4{1}_6{2}		0.070	115.1
IRR	130.2	3.84	52.7	T3	O8	T3	3{4}_4{24}_5{24}_6{18}_12{6}	5.37	3{1}_4{1}_5{1}	0.043	0.070	117.5
VSV	131	3.9	50	T1	O1	T3	3{8}_4{8}_5{16}_8{16}_9{32}	6.9	3{1}_9{8}	0.141	0.070	115.7
OSO	128.2	3.87	52.9	T1	O2	T2	3{6}_8{3}_14{15}	10.5	3{1}_8{1}_14{15}	0.142	0.072	115.3
ATS	142.5	4.06	37.7	T3	O6	T3	4{6}_6{16}_12{2}	6	6{3}_12{1}	0.141	0.072	115.3
MON	147.7	4.12	32.1	T1	O2	T1	4{4}_5{16}_8{12}	6	4{1}_5{2}_8{3}		0.073	116.0
GME	147.3	4.12	32.5	T1	O1	T1	4{18}_6{4}_8{6}	5.14	4{2}_6{1}	0.142	0.074	115.7
AFN	135.5	3.99	47.7	T2	O1	T4	4{22}_6{12}_8{32}	6.3	4{1}_6{2}_8{2}	0.06	0.074	111.6
RHO	147.1	4.12	32.9	T1	O1	T1	4{36}_6{8}_8{12}	5.14	4{1}_6{1}_8{1}		0.074	115.3
IWV	135.4	3.97	47	T1	O1	T2	4{32}_5{128}_6{48}_12{8}_14{40}	6.69	5{2}_12{1}_14{5}		0.074	113.5
AET	126.6	3.83	54.4	T1	O2	T5	4{16}_6{156}	5.81	4{1}_6{6}	0.123	0.075	116.7
SFF	132.4	3.92	49.4	T5	O14	T5	4{6}_5{24}_6{10}_10{2}	5.33	4{1}_6{1}_10{1}		0.075	114.9
-WEN	149.7	2.82	90	T3	O6	T2	4{12}_6{5}_8{6}_10{6}	6.41	8{4}_10{4}	0.143	0.075	154.5
TSC	142.4	4.06	37.8	T1	O2	T1	4{288}_6{96}_8{72}	5.05	4{2}_6{1}		0.075	115.2
FRA	156.5	4.11	30	T3	O13	T3	4{30}_6{40}	5.14	4{2}_6{1}	0.141	0.076	118.4
RUT	137.8	4	42.6	T2	O7	T3	4{12}_5{16}_6{12}_8{2}	5.14	4{1}_5{1}_6{1}		0.078	115.2
UEI	142.1	4.09	37.2	T2	O5	T2	4{28}_6{16}_8{44}	6.36	4{1}_6{1}_8{6}		0.081	113.7
AFI	148.5	4.13	31.3	T1	O3	T1	4{6}_6{52}	5.79	6{5}		0.084	116.0
SAT	142	4.06	38.3	T2	O7	T2	4{45}_6{30}_8{9}	5.14	4{2}_6{1}		0.084	114.8

FTC	T-O-T	b	omega	T1 label	O label	T2 label	ring-size{ring-number}:Ring Count (unit cell)	average ring size	ring index (this T-site)	BGB energy w.r.t. quartz (eV/TO2)	BS energy w.r.t. quartz (eV/TO2)	Eads (kJ/mol)
MFS	144.3	4.09	36.2	T2	O5	T6	4{4}_5{32}_6{4}_8{8}_10{4}	5.85	4{1}_5{1}_10{1}		0.084	114.6
GIS	149.8	4.14	30	T1	O2	T1	4{12}_8{8}	5.6	4{1}_8{3}		0.084	116.4
CGF	129.6	3.88	51.6	T3	O2	T5	4{20}_6{40}_8{6}_10{4}	5.83	4{1}_6{3}_10{1}		0.086	115.7
LTJ	137	3.95	41.8	T1	O2	T1	4{8}_6{12}_8{24}	6.73	4{2}_6{1}_8{4}	0.141	0.086	119.2
MTT	143.4	4.07	36.8	T3	O6	T7	5{8}_6{18}_10{2}	6	5{1}_10{1}		0.086	115.4
NON	144.4	4.1	35.6	T4	O9	T5	4{4}_5{64}_6{40}_12{8}	5.79	5{2}_6{2}_12{2}	0.035	0.087	114.4
ATO	142.5	4.07	37.7	T1	O3	T1	4{9}_6{42}	5.65	4{1}_6{2}		0.087	114.6
ABW	149.4	4.15	30.2	T1	O1	T1	4{2}_6{4}_8{2}	6	4{1}_8{1}		0.087	115.6
SIV	145.8	4.1	34	T2	O6	T2	4{48}_8{32}	5.6	4{1}_8{3}		0.089	115.7
IWW	136.4	3.99	45.2	T6	O16	T7	4{40}_5{56}_6{40}_8{16}_10{16}	6.76	4{1}_6{4}	0.132	0.089	113.7
RSN	131	3.9	50	T1	O1	T5	3{8}_4{10}_5{8}_6{8}_8{20}	6.98	3{1}_9{8}		0.091	115.7
ZON	131.9	3.92	49	T2	O5	T3	4{20}_6{24}_8{8}	5.54	4{1}_6{1}_8{1}	0.127	0.091	115.2
AEL	137.5	4	42.9	T1	O1	T2	4{8}_6{84}	5.83	4{1}_6{7}		0.091	115.0
SBN	132.4	3.91	50.6	T1	O2	T1	3{2}_4{6}_8{6}	5.57	3{1}_8{2}	0.134	0.092	114.5
FAR	139.5	4.04	41.5	T3	O8	T3	4{42}_6{56}	5.14	4{2}_6{1}		0.092	113.5
SFS	140.2	4.03	39.7	T2	O7	T5	4{10}_5{44}_6{18}_10{8}_12{6}	6.05	5{1}_6{3}_12{1}		0.092	115.6
DOH	157.4	4.23	22	T2	O4	T2	4{3}_5{30}_6{7}	5.1	4{1}_6{2}	0.155	0.092	117.1
JSW	132.9	3.92	48.6	T1	O4	T6	4{24}_6{40}_8{32}	6.17	4{2}_6{1}_8{3}		0.093	115.5
MAR	131.8	3.9	50.2	T2	O7	T3	4{36}_6{48}	5.14	4{1}_6{2}		0.093	115.5
DON	134.1	3.95	46.6	T1	O2	T4	4{16}_5{16}_6{68}	5.52	5{1}_6{3}		0.094	115.2
SAO	134.4	3.94	44.8	T1	O1	T3	4{40}_6{48}_12{34}	7.02	4{2}_6{1}_12{6}	0.133	0.095	117.4
SFG	142.6	4.05	37.9	T3	O11	T4	4{18}_5{26}_6{60}_7{8}_10{8}	5.82	6{4}_10{1}		0.095	115.8
NPT	131.7	3.91	51	T1	O3	T2	3{20}_4{3}_8{18}	5.27	3{1}_8{2}	0.129	0.096	114.2
YUG	144.5	4.09	35.6	T1	O3	T2	4{6}_5{8}_8{8}	5.82	4{1}_5{1}_8{2}		0.096	115.1
NPO	132.3	3.9	50.5	T1	O1	T1	3{2}_6{6}	5.25	3{1}_6{2}		0.097	115.3
OBW	131.9	3.9	51	T3	O3	T4	3{48}_4{2}_8{28}_10{8}	5.3	3{1}_8{2}		0.098	114.9
CZP	120.8	3.73	61.5	T1	O1	T3	4{18}_8{36}	6.67	4{2}_8{3}	0.109	0.098	117.4
IMF	142.8	4.06	37.4	T1	O16	T4	4{24}_5{256}_6{84}_10{72}_12{8}	6.07	5{2}_10{4}	0.146	0.099	115.6
CHA	147.8	4.13	32.1	T1	O1	T1	4{27}_6{6}_8{9}	5.14	4{2}_6{1}		0.099	115.3
AFT	146.5	4.11	33.4	Si3	O9	Si3	4{54}_6{12}_8{18}	5.14	4{2}_6{1}		0.101	115.6
ESV	139.1	4.02	41.5	T4	O10	T4	4{20}_5{16}_6{16}_8{4}	5.14	4{1}_6{2}	0.164	0.101	114.8
AFX	147.2	4.12	32.5	T2	O5	T2	4{36}_6{8}_8{12}	5.14	4{2}_6{1}	0.083	0.102	115.7
-ITV	148.1	2.81	74.3	T6	O15	T7	4{120}_6{132}	5.05	4{2}		0.102	168.3
STW	133.1	3.92	48.2	T1	O2	T2	4{36}_5{24}_8{6}_10{6}	5.17	5{1}_8{1}_10{1}	0.111	0.102	115.9
BEC	138.4	4.01	42.5	T1	O3	T1	4{14}_5{16}_6{8}_12{22}	7.47	4{2}_12{6}		0.102	114.6
OKO	139.1	3.99	39.9	Si3	O10	Si5	4{2}_5{72}_6{12}_10{4}_12{20}	6.55	5{4}_12{3}	0.165	0.102	118.2
STI	141.1	4.05	39.3	T2	O5	T3	4{32}_5{32}_6{32}_8{20}_10{8}	5.81	5{2}_8{1}		0.102	114.6
JRY	139.2	4	42.3	T1	O1	T1	4{8}_6{44}_10{28}	7.2	4{2}_6{6}		0.104	115.5
JSN	134.9	3.96	46.7	T2	O5	T3	4{10}_6{12}_8{4}	5.54	4{1}_6{1}_8{1}	0.159	0.105	114.5

FTC	T-O-T	b	omega	T1 label	O label	T2 label	ring-size{ring-number}:Ring Count (unit cell)	average ring size	ring index (this T-site)	BGB energy w.r.t. quartz (eV/TO2)	BS energy w.r.t. quartz (eV/TO2)	Eads (kJ/mol)
PON	134.3	3.94	47.4	T1	O3	T11	4{12}_6{28}_8{4}_10{20}	7	4{1}_6{3}_10{7}	0.137	0.105	115.2
SOF	139	4.03	41.5	T4	O8	T5	4{24}_5{16}_9{8}	5.17	5{2}_9{1}		0.106	114.1
AHT	125.5	3.81	55.5	T1	O1	T2	4{8}_6{52}	5.73	4{1}_6{6}		0.106	117.1
EZT	134.3	3.97	47.2	T1	O1	T5	4{28}_6{36}_8{4}_12{72}	8.74	4{1}_6{2}_8{1}_12{6}		0.106	113.4
MFI	132	3.92	48.7	T1	O2	T2	4{4}_5{88}_6{36}_10{28}	6.1	5{3}_10{3}		0.107	115.5
IFR	137.5	4	42.9	T1	O5	T3	4{14}_5{8}_6{20}_12{10}	6.46	6{4}_12{2}	0.162	0.107	115.0
PUN	127.2	3.8	56	T1	O1	T2	3{8}_4{20}_8{4}_10{12}	5.82	3{1}_4{1}_8{1}	0.159	0.108	117.4
KFI	147.7	4.13	32.1	T1	O2	T1	4{72}_6{16}_8{24}	5.14	4{2}_6{1}	0.165	0.108	115.3
MER	145.3	4.1	34.7	T1	O4	T1	4{24}_8{16}	5.6	4{1}_8{3}		0.108	115.2
VET	133	3.95	48.4	T3	O7	T4	5{8}_6{10}_7{4}_8{2}_12{1}	6.24	5{1}_6{3}_12{1}		0.109	113.7
SFE	136.9	3.98	44.1	T3	O6	T5	4{1}_5{4}_6{9}_12{1}	6	5{1}_6{2}_12{1}		0.109	115.3
MEP	146.2	4.12	33.7	T1	O1	T1	5{48}_6{6}	5.11	5{2}_6{1}		0.109	114.7
LOV	131.9	3.9	49.5	T2	O4	T2	3{4}_4{6}_6{8}_8{12}_9{16}	7.04	3{1}_8{6}		0.110	116.1
FER	150.1	4.15	29.9	T1	O1	T3	5{40}_6{2}_8{4}_10{8}_12{4}	6.41	5{3}_10{2}	0.169	0.110	115.8
BOZ	131.6	3.9	50.3	T2	O8	T3	3{56}_4{4}_6{4}_8{28}_10{12}	5.31	3{1}_8{2}	0.058	0.111	115.4
LTN	137.7	4	42.6	T2	O7	T3	4{432}_6{416}_8{48}	5.14	4{1}_6{2}	0.168	0.111	115.2
MTW	131.6	3.9	49.3	T3	O5	T7	4{2}_5{8}_6{22}_12{2}	6	5{1}_6{2}_12{1}	0.168	0.112	116.3
EUO	143.2	4.03	34.5	T9	O20	T9	4{8}_5{96}_6{44}_10{4}_12{24}	6.27	4{1}_5{2}	0.169	0.113	120.0
AFS	139	4.02	41.3	T1	O2	T2	4{42}_6{20}_8{24}_12{4}	5.87	4{1}_6{2}_8{2}_12{1}		0.113	115.0
NES	142.7	4.04	34.3	T6	O13	T7	4{12}_5{128}_6{48}_10{8}_12{40}	6.51	5{2}_6{2}_12{6}	0.169	0.113	119.5
-PAR	138.9	2.52	78.5	T4	O1	T1	4{12}_6{20}_8{16}_10{4}	6.46	6{3}_8{2}	0.171	0.114	184.2
LIO	132.1	3.92	48.5	T2	O7	T3	4{18}_6{24}	5.14	4{1}_6{2}		0.114	115.6
CAS	146.6	4.11	33.3	T1	O3	T3	5{8}_6{16}_8{4}	6	5{1}_6{2}_8{1}	0.17	0.114	115.7
MVY	130.4	3.86	52.1	T1	O2	T3	4{4}_6{20}_10{2}	6	4{1}_6{4}_10{1}		0.114	116.6
OWE	145.5	4.08	34.2	T2	O6	T2	4{10}_6{14}_8{14}	6.21	4{2}_8{2}		0.116	116.9
NSI	146.7	4.1	32.9	T1	O1	T3	5{4}_6{8}_8{2}	6	5{1}_6{2}_8{1}		0.116	116.7
STF	134.3	3.95	46.4	T1	O9	T3	4{6}_5{24}_6{10}_10{2}	5.33	5{2}_6{2}	0.178	0.117	115.4
MSE	139.6	4.03	41.7	T2	O7	T2	4{32}_5{72}_6{28}_10{8}	5.26	4{2}_6{1}		0.117	114.0
ATV	148.2	4.13	31.5	T1	O1	T1	4{4}_6{48}	5.85	4{1}_6{7}		0.118	115.8
CAN	142.6	4.07	37.6	T1	O3	T1	4{3}_6{8}	5.45	4{1}_6{1}	0.162	0.119	114.7
MOZ	138.9	4.01	43.1	T4	O7	T4	4{72}_6{30}_8{45}_12{1}	5.68	8{6}_12{1}		0.119	114.1
NAT	140.5	4.05	41	T1	O2	T1	4{20}_8{32}	6.46	4{3}_8{4}	0.179	0.119	113.2
-CHI	125	2.22	63.4	T3	O7	T4	4{8}_5{4}_6{20}_9{4}_10{4}	6.2	4{1}_9{1}_10{1}	0	0.119	217.0
AWW	141.9	4.06	38.4	T1	O3	T1	4{14}_6{12}_8{2}	5.14	4{1}_6{2}		0.120	114.7
TON	150.9	4.15	29	T2	O4	T3	5{8}_6{18}_10{2}	6	5{1}_10{1}	0.132	0.121	116.6
SSY	134.8	3.94	46.7	T3	O4	T4	4{2}_5{8}_6{18}_12{2}	6	5{1}_12{1}	0.169	0.123	115.8
RTH	138	4	42.3	T2	O5	T4	4{14}_5{16}_6{4}_8{4}	5.05	4{1}_5{1}_8{1}	0.161	0.124	115.5
-SVR	140.6	2.83	80.5	T4	O11	T5	4{4}_5{76}_6{16}_10{20}_11{4}	6.67	5{2}_6{1}_12{1}		0.124	161.8
IHW	131.9	3.89	49.9	T7	O17	T8	4{4}_5{96}_6{48}_8{8}_12{32}	6.55	5{2}_6{2}		0.124	116.5

FTC	T-O-T	b	omega	T1 label	O label	T2 label	ring-size{ring-number}:Ring Count (unit cell)	average ring size	ring index (this T-site)	BGB energy w.r.t. quartz (eV/TO2)	BS energy w.r.t. quartz (eV/TO2)	Eads (kJ/mol)
UWY	133.2	3.93	48.4	T8	O21	T9	4{23}_5{20}_6{40}_10{18}	6.06	4{1}_6{4}	0.173	0.125	115.0
FAU	142	4.06	38.2	T1	O4	T1	4{144}_6{64}_12{16}	5.14	4{1}_6{1}_12{1}	0.189	0.126	114.9
SGT	136.3	3.98	44.3	T1	O1	T2	4{12}_5{48}_6{16}	5.05	5{2}_6{1}		0.126	115.1
OSI	135.7	3.99	46.8	T1	O1	T1	4{6}_6{32}_12{2}	6	4{1}_6{1}		0.127	112.4
BOG	136.2	3.98	44.1	T3	O9	T5	4{36}_6{8}_8{48}_10{18}	6.87	4{1}_5{1}_6{2}_10{2}		0.129	115.3
SBT	135.9	3.97	44.7	T2	O9	T3	4{108}_6{84}_8{99}_12{60}	6.97	4{1}_6{2}_8{4}_12{6}		0.129	115.5
TOL	127.1	3.83	56.2	T2	O7	T3	4{36}_6{48}	5.14	4{1}_6{2}	0.183	0.132	115.2
SBE	139.5	4.03	40.9	T4	O10	T3	4{96}_6{64}_8{120}_12{8}	6.33	4{1}_6{2}_8{6}_12{1}		0.132	114.6
AEN	128.2	3.82	50.4	T3	O9	T3	4{12}_6{80}_8{12}	6	4{1}_6{5}	0.173	0.133	120.7
AEI	146.1	4.11	33.8	T1	O1	T1	4{36}_6{8}_8{12}	5.14	4{2}_6{1}	0.177	0.133	115.2
JOZ	131.3	3.87	51.1	T1	O1	T2	3{8}_4{4}_8{12}	5.67	3{1}_4{1}_8{1}	0.165	0.135	116.8
CON	137.2	3.99	43.3	T2	O5	T4	4{22}_5{24}_6{28}_10{16}_12{26}	7.31	4{1}_5{1}_6{2}_10{2}_12{1}		0.135	115.3
GIU	138.1	4.02	43.5	T4	O3	T4	4{48}_6{64}	5.14	4{2}_6{1}		0.135	113.1
APD	143.7	4.08	36.7	T1	O3	T1	4{12}_6{48}_8{24}	6.29	4{1}_6{4}_8{5}	0.15	0.136	114.8
MTF	135.6	3.96	45.7	T4	O11	T5	4{2}_5{32}_6{14}_7{8}_8{6}	5.74	6{3}_7{2}	0.187	0.136	115.3
LEV	142.7	4.06	37.6	T1	O1	T1	4{36}_6{18}_8{9}	5.14	4{2}_6{1}		0.138	115.4
SAF	137.3	3.98	44	T1	O1	T1	4{12}_6{136}	5.84	4{1}_6{7}		0.138	115.4
VNI	131.3	3.9	50	T3	O7	T4	3{12}_4{12}_5{32}_8{48}	6.04	3{1}_8{4}		0.141	115.7
APC	134	3.95	46.9	T1	O1	T1	4{20}_6{8}_8{20}	6	4{1}_8{3}		0.141	115.0
JSR	126.2	3.77	56.4	Si1	O1	Si3	3{48}_4{24}_6{12}_11{24}	5.33	3{1}_4{1}_6{1}	0.155	0.141	119.0
IFO	132.8	3.92	51	Si1	O3	Si1	4{10}_6{52}_16{2}	6	6{6}		0.142	113.5
ITT	132.7	3.92	51	Si3	O7	Si3	3{2}_4{18}_5{24}_6{18}_10{6}	5.38	3{1}_5{2}	0.201	0.142	113.5
GON	141.4	4.06	38.1	T1	O1	T4	4{4}_5{8}_6{24}_12{2}	5.89	5{1}_6{3}_12{1}	0.165	0.143	115.0
IWS	135.6	3.99	46.6	T2	O15	T5	4{66}_5{48}_6{64}_12{40}	6.28	5{1}_6{2}_12{3}		0.143	112.5
UOS	144.3	4.08	35.8	T1	O4	T3	4{12}_5{8}_6{4}_8{8}_10{8}	6.4	5{1}_6{1}_8{2}_10{2}	0.17	0.143	115.6
PHI	145.1	4.1	34.9	T2	O6	T2	4{24}_8{16}	5.6	4{2}_8{1}	0.105	0.147	115.0
BOF	142	4.06	38.4	T1	O2	T2	4{8}_5{8}_6{16}_10{4}	5.78	5{2}_6{2}_10{1}	0.195	0.153	114.7
AWO	139.4	4.03	40.9	T1	O3	T3	4{28}_6{16}_8{44}	6.36	4{2}_8{2}		0.153	114.6
SFN	134.9	3.94	46.9	T3	O7	T8	4{4}_5{8}_6{22}_14{2}	6	5{1}_14{1}		0.154	115.6
AFY	128.3	3.86	54	T1	O2	T1	4{15}_8{3}_12{1}	5.05	4{1}_8{1}_12{1}		0.154	115.0
WEI	130.9	3.9	50	T1	O1	T2	3{8}_4{4}_6{4}_8{4}_10{4}	5.67	3{1}_6{1}_10{1}	0.205	0.155	115.7
AST	148.3	4.13	31.5	T1	O1	T1	4{24}_6{24}	5	4{2}_6{1}	0.208	0.156	115.8
MOR	147.6	4.12	32.2	T1	O1	T1	4{4}_5{48}_8{12}_12{4}	5.88	5{2}_8{1}_12{1}		0.159	115.9
LAU	141.9	4.06	38.2	T2	O6	T3	4{12}_6{24}_10{8}	6.18	4{1}_6{4}_10{2}		0.159	114.9
RWY	116.1	3.5	73.1	T1	O3	T1	3{48}_8{6}_12{8}	4.65	3{2}_12{1}		0.160	123.1
SZR	149.2	4.14	30.1	T1	O1	T1	4{12}_5{16}_6{8}_8{12}_10{12}	6.53	4{1}_6{2}_10{3}		0.160	116.3
SBS	135.8	3.97	44.7	T1	O1	T2	4{72}_6{56}_8{66}_12{40}	6.97	4{1}_6{2}_8{4}_12{6}		0.162	115.5
SFH	136.5	3.96	44.5	T4	O10	T7	4{8}_5{16}_6{44}_14{4}	6	5{1}_14{1}		0.164	116.3
BRE	139.9	4.03	40.4	T1	O4	T3	4{6}_5{8}_6{2}_8{4}	5.4	4{1}_5{1}_8{2}		0.165	115.1

FTC	T-O-T	b	omega	T1 label	O label	T2 label	ring-size{ring-number}:Ring Count (unit cell)	average ring size	ring index (this T-site)	BGB energy w.r.t. quartz (eV/TO2)	BS energy w.r.t. quartz (eV/TO2)	Eads (kJ/mol)
AFG	139.1	4.02	41.5	T1	O3	T1	4{24}_6{32}	5.14	4{2}_6{1}	0.211	0.168	114.8
DAC	143.7	4.08	36.2	T2	O7	T4	4{2}_5{24}_8{4}_10{8}	6.32	5{3}_8{1}_10{2}		0.169	115.2
USI	133.2	3.94	48.5	T2	O5	T3	4{26}_6{40}_10{4}_12{8}	6.15	4{2}_6{1}_12{2}		0.169	114.3
LOS	139.1	4.02	41.6	T1	O1	T1	4{12}_6{16}	5.14	4{2}_6{1}	0.206	0.169	114.7
PCR	141.1	4.06	39.1	T1	O1	T7	5{56}_6{20}_8{4}_10{24}_12{4}	6.67	5{3}_6{1}_10{2}		0.170	114.1
BCT	160.1	4.22	19.1	T1	O2	T1	4{2}_6{8}	5.6	4{1}_6{2}		0.170	120.2
CGS	138.8	4.02	41.6	T3	O9	T4	4{24}_6{4}_8{32}_10{4}	6.5	4{1}_8{5}_10{1}	0.208	0.170	114.7
SFV	134.1	3.94	45.7	T1	O4	T6	{107}_5{632}_6{240}_8{106}_10{18}	6.12	10{1}	0.198	0.171	116.6
UTL	130.1	3.89	53	T1	O1	T7	4{12}_5{72}_6{12}_12{4}_14{20}	6.73	5{2}_12{1}_14{5}		0.181	113.9
LTA	145.2	4.1	34.8	Si1	O2	Si1	4{18}_6{8}_8{3}	4.97	4{2}_6{1}	0.23	0.181	115.1
MEL	141.2	4.04	38.9	T3	O9	T3	4{10}_5{80}_6{32}_8{12}_10{24}	6.13	5{2}_10{4}		0.187	115.6
DFO	133.8	3.95	46	T1	O1	T1	4{84}_6{144}_8{6}_10{6}_12{3}	5.53	4{2}_12{1}		0.189	115.7
IWR	139	4.03	43	T4	O3	T4	4{26}_5{16}_6{32}_10{16}_12{32}	7.54	4{1}_6{4}		0.190	112.9
BSV	130.1	3.88	52.8	T1	O1	T1	4{72}_6{16}_12{2352}	11.72	4{2}_12{147}		0.193	114.7
-LIT	145.6	2.48	49.2	T1	O3	T2	4{8}_6{8}_8{12}	6.29	4{1}_6{1}_8{1}	0.174	0.194	211.5
DDR	138.2	4.03	42.9	T1	O3	T1	4{18}_5{108}_6{6}_8{9}	5.11	4{1}_5{2}		0.194	113.0
CDO	147.8	4.06	32.8	T2	O6	T2	5{40}_8{12}	5.69	5{2}	0.074	0.199	119.4
SAV	143.2	4.11	37.3	T1	O9	T1	4{36}_6{8}_8{12}	5.14	4{1}_8{2}	0.199	0.209	112.3
ASV	132.9	3.97	48.5	T1	O1	T2	4{12}_6{12}_12{28}	8.77	6{3}_12{14}		0.221	112.3
UFI	137.3	3.96	42.4	T2	O6	T2	4{36}_5{16}_6{16}_8{8}	5.05	4{1}_5{1}_8{1}	0.224	0.222	118.1
EON	140.2	4.04	41.3	T1	O10	T1	4{20}_5{36}_6{2}_8{18}_12{4}	5.8	4{2}_12{1}	0.233	0.228	113.6
HEU	139.9	4.03	40.1	T1	O1	T5	4{12}_5{24}_8{6}_10{4}	5.57	5{3}_10{1}	0.257	0.233	115.3
BPH	138.8	4.02	41.4	T1	O1	T2	4{21}_6{10}_8{12}_12{2}	5.87	4{1}_6{2}_8{2}_12{1}		0.234	114.9
THO	140.3	4.08	40	T1	O2	T2	4{10}_8{18}	6.57	4{3}_8{5}	0.253	0.234	112.0
ACO	148.4	4.13	31.5	T1	O2	T1	4{12}_8{12}	6	4{2}_8{2}	0.229	0.238	115.8
STT	129.1	3.86	51.7	T3	O1	T4	4{24}_5{32}_6{16}_7{4}_9{4}	5.2	5{2}_6{1}	0	0.257	117.0
LTF	140.9	4.04	39.6	T1	O2	T2	4{60}_5{24}_6{12}_8{36}_12{2}	5.55	4{2}_8{1}	0.25	0.275	115.1
ITH	141.5	4.05	39.2	T6	O3	T7	4{18}_5{20}_6{40}_9{8}_10{8}	6	5{2}_9{2}_10{1}	0.293	0.286	114.7
UOZ	132.9	3.93	48.5	T2	O4	T4	4{24}_6{24}_12{28}	7.58	6{3}_12{14}		0.319	115.0
SOD	160.3	4.23	19.2	T1	O1	T1	4{6}_6{8}	5.14	4{1}_6{2}	0.282	0.331	119.5
SFW	145.9	4.11	34	Si1	O3	Si1	4{81}_6{18}_8{27}	5.14	4{2}_6{1}	0.339	0.334	115.1
CFI	137.5	4.02	44.8	T1	O6	T1	4{2}_5{12}_6{20}_14{2}	6	4{1}_5{1}	0.358	0.363	112.0
MSO	144.8	4.09	35.2	T2	O8	T2	4{36}_6{93}	5.44	4{1}_6{3}		0.407	115.4
EPI	136.5	3.98	44.3	T1	O1	T3	4{2}_5{24}_8{4}_10{8}	6.32	5{3}_8{1}_10{2}		0.419	115.1
BIK	150.6	4.15	29	T1	O3	T1	5{4}_6{8}_8{2}	6	5{1}_8{1}	0.403	0.451	116.6
MAZ	140.6	4.04	39.6	T1	O3	T1	4{18}_5{12}_6{2}_8{12}_12{2}	5.74	4{2}_12{1}		0.455	115.1
ANA	148.8	4.13	31.2	T1	O1	T1	4{24}_6{16}_8{96}	7.06	4{1}_6{1}_8{8}		0.477	116.1
MRE	141.4	4.02	39.3	T3	O1	T3	4{4}_5{16}_6{60}	5.7	6{4}		0.509	116.6
LTL	138.2	4	42.8	T2	O5	T2	4{24}_6{10}_8{18}_12{1}	5.89	8{6}_12{1}	0.482	0.523	115.0

FTC	T-O-T	b	omega	T1 label	O label	T2 label	ring-size{ring-number}:Ring Count (unit cell)	average ring size	ring index (this T-site)	BGB energy w.r.t. quartz (eV/TO2)	BS energy w.r.t. quartz (eV/TO2)	Eads (kJ/mol)
MWW	141.1	4.05	39.8	T1	O3	T4	4{24}_5{48}_6{38}_10{18}	5.81	5{2}_6{2}_10{2}		0.538	114.2
EDI	140.4	4.03	40	T1	O2	T1	4{5}_8{9}	6.57	4{3}_8{5}		0.568	115.4
ETR	137.3	3.98	44	Si1	O1	Si3	4{36}_6{8}_8{48}_10{18}	6.87	4{1}_8{5}_10{5}		0.618	115.4
ERI	142.1	4.06	38.1	T1	O3	T1	4{24}_6{12}_8{6}	5.14	4{2}_6{1}	0.574	0.648	115.0
TER	142.9	4.07	37.5	T2	O5	T7	4{16}_5{48}_6{56}_10{36}	6.41	5{1}_6{2}_10{3}	1.075	1.105	114.8
RRO	127.1	3.82	55.7	T2	O6	T4	4{6}_5{12}_8{2}_10{8}	6.43	4{1}_5{1}_8{1}_10{1}			116.3
TUN	142.3	4.05	37.4	T8	O34	T8	4{20}_5{168}_6{52}_8{12}_10{36}	6.24	6{3}_8{1}_10{2}			116.2
PAU	146.6	4.11	33.4	T1	O1	T7	4{504}_6{24}_8{300}	5.51	4{2}_8{1}			115.6
EAB	144.1	4.08	35.9	T1	O2	T1	4{24}_6{12}_8{6}	5.14	4{2}_6{1}			115.5
STO	139.6	4.01	41.5	T5	O39	T5	4{22}_5{32}_6{130}_8{4}	5.64	6{4}_8{1}			115.5
RTE	143	4.07	36.9	T2	O5	T3	4{10}_5{8}_6{8}_8{2}	5.14	4{1}_5{1}_6{1}			115.3
SFO	141.5	4.05	38.9	T1	O6	T3	4{22}_6{24}_8{4}_12{2}	5.54	4{2}_6{3}			115.0
ITR	142.4	4.06	38.2	T1	O4	T3	4{36}_5{40}_6{80}_9{16}_10{16}	6	5{2}_9{2}_10{1}			114.9
SVV	137.7	4	43.2	Si3	O7	Si4	4{24}_5{16}_6{24}_8{2}	5.09	4{1}_5{1}_6{1}			114.7
ISV	137.8	4	43.4	T2	O7	T2	4{28}_5{32}_6{16}_12{36}	7.14	4{2}_6{1}_12{1}			114.5
SEW	136.1	3.97	46.7	Si6	O22	Si6	4{26}_5{22}_6{38}_10{4}_12{4}	5.64	4{2}_6{1}			113.8
ITE	137.8	4.05	42.5	T2	O7	T4	4{28}_5{32}_6{8}_8{8}	5.05	4{1}_5{1}_8{1}			112.0