Electronic Supplementary Information

Interfacial catalysis in and initial reaction mechanism of Al2O3 films fabricated by atomic layer deposition using non-hydrolytic sol-gel chemistry

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Table S1 The atomic coordinates of all stationary points.

OH-terminated Si(001) substrate, $Si_{63}H_{48}$-$(OH)_{16}$				
Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84009900	-0.61490100
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61489900
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84009900	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280100
Si	-1	-5.76009800	0.00000200	0.74280100
Si	-1	-5.76009900	-3.84010200	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000100	7.68020000	0.74279900
Si	-1	-1.91999900	3.84010000	0.74280100
Si	-1	-1.92000200	0.00000000	0.74279800

Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000200	-7.68020000	0.74279900
Si	-1	1.92000000	7.68020000	0.74280100
Si	-1	1.92000200	3.84010100	0.74280000
Si	-1	1.92000100	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000100	-7.68020000	0.74280000
Si	-1	5.76009700	7.68020000	0.74279900
Si	-1	5.76009800	3.84010000	0.74279600
Si	-1	5.76009900	0.00000000	0.74280000
Si	-1	5.76009900	-3.84010200	0.74279900
Si	-1	5.76010000	-7.68019900	0.74279900
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000

H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180100
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90149900	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620100	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01329900
H	-1	7.05950100	3.84760000	0.03180300
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960100	-3.84790000	0.03190100
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.02296600	5.74433400	1.96473200
Si	0	-5.04957500	1.94624500	1.93566100
Si	0	-5.03619200	-1.93915600	1.93267000
Si	0	-5.03373000	-5.74021400	1.96493900
Si	0	-2.59392100	5.75698300	1.95405500
Si	0	-2.62851300	1.91891700	1.93061500
Si	0	-2.61072200	-1.91833800	1.93985400
Si	0	-2.60975200	-5.75471000	1.94408900
Si	0	2.60967600	5.75473500	1.94412500
Si	0	2.61066500	1.91830200	1.93989700
Si	0	2.62856600	-1.91900300	1.93061300
Si	0	2.59391600	-5.75710300	1.95396700
Si	0	5.03362300	5.74010300	1.96494400
Si	0	5.03610700	1.93926500	1.93262300
Si	0	5.04967500	-1.94621500	1.93569600
Si	0	5.02290200	-5.74433000	1.96476600

O	0	-5.33998300	5.57877100	3.61248300
O	0	-5.40519400	2.17274800	3.56529100
O	0	-5.35029100	-2.05615400	3.58593100
O	0	-5.36983300	-5.48741600	3.59726100
O	0	-2.18262200	5.74773700	3.58010000
O	0	-2.41863000	1.90676500	3.60213000
O	0	-2.23394500	-1.92135600	3.57493700
O	0	-2.36654800	-5.75140300	3.61077600
O	0	2.36648700	5.75105200	3.61076100
O	0	2.23433700	1.92195400	3.57507300
O	0	2.41886500	-1.90661100	3.60217000
O	0	2.18236900	-5.74845000	3.57997100
O	0	5.36955000	5.48639300	3.59726700
O	0	5.34991000	2.05745000	3.58584100
O	0	5.40549200	-2.17245100	3.56529000
O	0	5.33945800	-5.57824900	3.61253600
H	0	-5.64559300	4.69449400	3.86150400
H	0	-4.67748900	1.88627500	4.13816800
H	0	-5.68112900	-2.92370200	3.85988000
H	0	-4.60892000	-5.70322800	4.15808100
H	0	-2.96721000	5.67868100	4.14422700
H	0	-1.51898100	1.86624200	3.94705000
H	0	-3.03483800	-1.94974700	4.12016900
H	0	-1.46271500	-5.66270500	3.93573900
H	0	1.46279100	5.66218300	3.93600400
H	0	3.03550700	1.95045900	4.11993400
H	0	1.51929600	-1.86543800	3.94724900
H	0	2.96678300	-5.67709700	4.14405300
H	0	4.60851400	5.70204200	4.15800900
H	0	5.67986800	2.92553400	3.85927500
H	0	4.67777600	-1.88587300	4.13811600
H	0	5.64705300	-4.69460700	3.86129400

Cl-Al-terminated surface

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000

Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490100
Si	-1	-3.84009900	3.84010000	-0.61490100
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020100	-0.61489800
Si	-1	0.00000000	3.84009800	-0.61489500
Si	-1	0.00000000	-0.00000100	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84009900	3.84010000	-0.61490100
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280100
Si	-1	-5.76010100	3.84009900	0.74280200
Si	-1	-5.76009800	0.00000100	0.74280000
Si	-1	-5.76010000	-3.84009900	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000300	7.68019800	0.74279900
Si	-1	-1.92000500	3.84010200	0.74279700
Si	-1	-1.91999800	-0.00000100	0.74280000
Si	-1	-1.92000100	-3.84010100	0.74280000
Si	-1	-1.91999900	-7.68020000	0.74280000
Si	-1	1.92000300	7.68019800	0.74279900
Si	-1	1.92000600	3.84010200	0.74279700
Si	-1	1.91999800	-0.00000100	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000

Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84009900	0.74280200
Si	-1	5.76009800	0.00000100	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87799900	8.93300000	1.52980000

H	-1	-7.05960000	3.84790100	0.03189900
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90149800	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90149800	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87619900	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760100	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-4.95954500	5.75339800	2.02298800
Si	0	-5.05774300	1.92354700	1.91026700
Si	0	-4.95543900	-1.92960800	1.99373500
Si	0	-5.04346800	-5.75677500	1.94073600
Si	0	-2.43582900	5.75523300	1.99686400
Si	0	-2.62460000	1.92300500	1.92587800
Si	0	-2.43377100	-1.92082700	1.98131700
Si	0	-2.60885900	-5.74320400	1.93933800
Si	0	2.43598600	5.75522700	1.99682400
Si	0	2.62457800	1.92300800	1.92582500
Si	0	2.43370300	-1.92082700	1.98126700
Si	0	2.60876100	-5.74321900	1.93936900
Si	0	4.95968700	5.75333900	2.02286200
Si	0	5.05772900	1.92356400	1.91028300
Si	0	4.95546100	-1.92957500	1.99375300
Si	0	5.04335900	-5.75682600	1.94087500
O	0	-5.32130300	5.60356100	3.65367500
O	0	-5.28416400	1.94638000	3.57826500
O	0	-5.27833300	-1.99303800	3.64151600
O	0	-5.25522800	-5.64656800	3.60881600
O	0	-1.53355600	5.72164100	3.40273300
O	0	-2.42075400	1.94773900	3.59897900

O	0	-1.54305000	-1.92894200	3.39512900
O	0	-2.39408000	-5.63056600	3.60730400
O	0	1.53389300	5.72166500	3.40281200
O	0	2.42064100	1.94789600	3.59895200
O	0	1.54240000	-1.92891500	3.39473100
O	0	2.39388300	-5.63083200	3.60733600
O	0	5.32137600	5.60354900	3.65355700
O	0	5.28407400	1.94654500	3.57826900
O	0	5.27846500	-1.99289500	3.64152000
O	0	5.25506100	-5.64678200	3.60898400
H	0	-6.22520100	5.36927300	3.88994800
H	0	-6.19232900	-2.11113400	3.92303500
Al	0	-3.86070900	1.99665200	4.54133400
Al	0	-3.82639100	-5.45287800	4.54263300
Cl	0	-3.89563800	2.07605500	6.60588900
Cl	0	-3.83999700	-5.15959200	6.58904400
Al	0	-0.00022000	-1.97175000	4.13556000
Al	0	0.00015400	5.53762000	4.13302200
Cl	0	0.00012200	-2.06998000	6.21132100
Cl	0	0.00008700	5.13448500	6.17240800
Al	0	3.82616000	-5.45351700	4.54278300
Al	0	3.86057800	1.99700800	4.54130000
Cl	0	3.83939300	-5.16134900	6.58936000
Cl	0	3.89623900	2.07709500	6.60581900
H	0	6.22521100	5.36908200	3.88985800
H	0	6.19247100	-2.11107300	3.92301700

Im1$^{A\text{-}Si}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000

Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010100	3.84010100	-0.61490000
Si	-1	-3.84010000	-0.00000100	-0.61490000
Si	-1	-3.84009900	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61489900
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68019900	0.74280100
Si	-1	-5.76009900	3.84009900	0.74280000
Si	-1	-5.76010100	-0.00000100	0.74279900
Si	-1	-5.76010000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000100	7.68020000	0.74280100
Si	-1	-1.91999900	3.84010100	0.74279900
Si	-1	-1.92000000	0.00000100	0.74279900
Si	-1	-1.92000200	-3.84009900	0.74280100
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000

H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000

H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.02054400	5.74767200	1.97108700
Si	0	-5.08591700	1.93164400	1.95964300
Si	0	-5.05100600	-1.92194000	1.95479500
Si	0	-5.03494100	-5.74639000	1.96470000
Si	0	-2.58793300	5.75702000	1.95612200
Si	0	-2.60590100	1.91532700	1.96015800
Si	0	-2.58428300	-1.92325900	1.95697700
Si	0	-2.61128400	-5.75561300	1.94309300
Si	0	2.60993900	5.75503700	1.94458300
Si	0	2.60447000	1.91899400	1.93902300
Si	0	2.62347800	-1.92001400	1.93099300
Si	0	2.59472900	-5.75660000	1.95434900
Si	0	5.03408500	5.74010200	1.96464800
Si	0	5.03400700	1.93898700	1.93822500
Si	0	5.04668500	-1.94621200	1.93710600
Si	0	5.02338600	-5.74460800	1.96409500
O	0	-5.32869700	5.60769900	3.62389200
O	0	-5.75219200	2.10242000	3.49155500
O	0	-5.59753700	-1.86280200	3.54335000
O	0	-5.35941500	-5.53599800	3.60089900
O	0	-2.14284800	5.74489000	3.57291200
O	0	-2.07107600	1.86335800	3.56251300
O	0	-1.95811200	-1.98816700	3.51523800
O	0	-2.36927400	-5.75043900	3.60872000
O	0	2.36786900	5.75465500	3.61129000
O	0	2.18375800	1.93755300	3.56503600
O	0	2.39403800	-1.91383800	3.59927600
O	0	2.18821900	-5.74025300	3.58126200

O	0	5.37016300	5.48727600	3.59690600
O	0	5.35572400	2.05332900	3.58882800
O	0	5.40483900	-2.17561000	3.56613900
O	0	5.34012900	-5.57968400	3.61205500
H	0	-5.78003700	4.79498200	3.88892500
H	0	-5.78920300	1.29492900	4.02079800
H	0	-5.63685400	-2.72269600	3.98372900
H	0	-4.57868400	-5.71852700	4.14635100
H	0	-2.90937300	5.69799300	4.16258500
H	0	-1.14343200	2.10586700	3.68855200
H	0	-2.13364600	-1.19995100	4.04692900
H	0	-1.48429800	-5.55895700	3.94038700
H	0	1.46275900	5.69222000	3.93884000
H	0	2.96396200	1.93834500	4.13910500
H	0	1.48705100	-1.95912800	3.92515800
H	0	2.97550300	-5.68261200	4.14304900
H	0	4.61105700	5.70735500	4.15850000
H	0	5.67744300	2.92366300	3.86469000
H	0	4.68041500	-1.88978200	4.14303000
H	0	5.64525400	-4.69542400	3.86168800
Si	0	-3.18445300	1.66265600	6.44181000
Cl	0	-1.15747500	1.50340900	6.50416100
Cl	0	-3.98835600	0.10644800	5.38140500
Cl	0	-3.87757000	1.49458000	8.34913600
Cl	0	-3.78018600	3.46176900	5.72303200

TS1$^{A\text{-}Si}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000

Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76010000	0.00000000	0.74280000
Si	-1	-5.76010000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000

H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000

H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.06286300	5.75052000	1.99464200
Si	0	-5.13579200	1.94833000	1.95817700
Si	0	-5.05954000	-1.93057300	1.96618200
Si	0	-5.02906900	-5.74538900	1.95915100
Si	0	-2.61179600	5.72163200	1.95430700
Si	0	-2.68277200	1.95510800	1.91196400
Si	0	-2.59057300	-1.96120300	1.96451900
Si	0	-2.60351100	-5.74376400	1.94983500
Si	0	2.59973700	5.74629400	1.95126700
Si	0	2.60557900	1.93336900	1.94496500
Si	0	2.61894900	-1.91829800	1.93178600
Si	0	2.60135800	-5.75173100	1.95526400
Si	0	5.02718800	5.74396800	1.95982700
Si	0	5.06147600	1.92846300	1.95216300
Si	0	5.04676000	-1.94478500	1.93693800
Si	0	5.02836600	-5.74643100	1.95974600
O	0	-5.52717400	5.65052600	3.59733800
O	0	-5.74278000	2.22358200	3.49057300
O	0	-5.60803000	-1.90970900	3.54657100
O	0	-5.35429700	-5.51207600	3.59484000
O	0	-2.02499700	5.31084200	3.49792600
O	0	-2.10733800	2.44723700	3.57672400
O	0	-1.94234200	-2.26962300	3.48869000
O	0	-2.27186800	-5.65410700	3.59691000
O	0	2.27788500	5.69667100	3.60109200
O	0	2.02198100	2.12283500	3.50695900
O	0	2.34120200	-1.86878600	3.59574600
O	0	2.22698200	-5.67184200	3.58617400
O	0	5.34867800	5.51255300	3.59618800

O	0	5.57243000	1.93574200	3.54539500
O	0	5.41028700	-2.19585100	3.56169100
O	0	5.34674700	-5.59572600	3.60829700
H	0	-5.68886300	4.74981800	3.91489600
H	0	-5.55760500	1.54892300	4.15896100
H	0	-5.70859000	-2.78338400	3.94880300
H	0	-4.57937600	-5.71019500	4.14279100
H	0	-2.42218800	5.73263400	4.27136000
H	0	-1.80511100	3.39148800	3.55423900
H	0	-2.24105200	-1.67930300	4.19474200
H	0	-1.82556500	-4.84256600	3.87536100
H	0	1.75224600	4.94817200	3.91307200
H	0	2.21162900	1.41971900	4.13996100
H	0	1.52700300	-2.27721300	3.91410500
H	0	3.02232000	-5.73600700	4.13623100
H	0	4.57447500	5.71411000	4.14404100
H	0	5.64741500	2.81875700	3.93272600
H	0	4.71246100	-1.88028600	4.15404000
H	0	5.63533600	-4.70884900	3.86871200
Cl	0	-0.44646800	3.07069200	5.59120200
Si	0	-2.24147200	1.95368000	5.36195700
Cl	0	-3.72217700	3.26630100	5.95413500
Cl	0	-1.77754800	0.72813000	7.00638600
Cl	0	-3.42930300	0.30684400	4.52306300

Im2$^{A\text{-}Si}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000

Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010100	-0.61490100
Si	-1	0.00000000	0.00000000	-0.61489900
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010100	-0.61489900
Si	-1	3.84010000	0.00000100	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76009900	7.68020000	0.74280000
Si	-1	-5.76010000	3.84009900	0.74280000
Si	-1	-5.76010000	0.00000100	0.74280100
Si	-1	-5.76010100	-3.84009900	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000100	0.00000000	0.74279900
Si	-1	-1.92000000	-3.84010100	0.74280000
Si	-1	-1.91999800	-7.68020000	0.74280100
Si	-1	1.91999800	7.68020100	0.74280100
Si	-1	1.92000300	3.84009600	0.74280000
Si	-1	1.91999600	-0.00000100	0.74279900
Si	-1	1.92000100	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76009900	7.68019900	0.74280000
Si	-1	5.76010100	3.84010300	0.74279900
Si	-1	5.76010000	0.00000000	0.74280200
Si	-1	5.76010100	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000

H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150100	-8.88670000	1.61880000
H	-1	1.90150100	8.88670000	1.61880000

H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84759900	0.03180000
H	-1	7.05810000	0.00000000	0.02889900
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.07125400	5.75194700	1.99070700
Si	0	-5.12534900	1.95079500	1.96608300
Si	0	-5.06226500	-1.93263300	1.96923200
Si	0	-5.02801800	-5.74530700	1.95879800
Si	0	-2.62272600	5.71966700	1.94227700
Si	0	-2.68221000	1.95972400	1.89619900
Si	0	-2.59122800	-1.96898000	1.97013800
Si	0	-2.60255900	-5.74179700	1.94969300
Si	0	2.59467500	5.74228500	1.95385100
Si	0	2.59727000	1.93657200	1.95230400
Si	0	2.61406900	-1.91838900	1.93510800
Si	0	2.60081800	-5.75284400	1.95567700
Si	0	5.02422300	5.74483100	1.96010500
Si	0	5.05900500	1.92642800	1.95416900
Si	0	5.04490900	-1.94455200	1.93889800
Si	0	5.02786800	-5.74603900	1.95967200
O	0	-5.54214600	5.64672800	3.59113300
O	0	-5.65768100	2.24102400	3.52504700
O	0	-5.63615100	-1.91559900	3.53869400
O	0	-5.35122100	-5.51368500	3.59528200
O	0	-2.03738100	5.26016500	3.48155100
O	0	-2.12523700	2.51820700	3.58478300
O	0	-1.93480000	-2.32428900	3.47729500
O	0	-2.26731700	-5.63855300	3.59471600
O	0	2.25229600	5.67743200	3.59850300
O	0	2.00007300	2.16756100	3.50058600
O	0	2.32041400	-1.86841400	3.59463400
O	0	2.22752900	-5.68432100	3.58648800
O	0	5.34489500	5.52616200	3.59776500
O	0	5.59012400	1.91282700	3.53954800

O	0	5.41912500	-2.19878200	3.56058100
O	0	5.34685200	-5.59307900	3.60788400
H	0	-5.72701700	4.74653600	3.89585200
H	0	-5.41951200	1.56795000	4.18064800
H	0	-5.71102100	-2.78848300	3.94803300
H	0	-4.57134000	-5.70212400	4.13976500
H	0	-2.26821500	5.77633300	4.26434200
H	0	-1.91345100	3.50101700	3.59718900
H	0	-2.16708400	-1.69947500	4.17999000
H	0	-1.84453600	-4.80985800	3.86192100
H	0	1.78671400	4.88538200	3.90327300
H	0	1.95273500	1.41897400	4.10874400
H	0	1.48008600	-2.23530400	3.89646800
H	0	3.02487600	-5.72735800	4.13564900
H	0	4.56748100	5.72080900	4.14330600
H	0	5.62080700	2.78375400	3.95787700
H	0	4.74748000	-1.84860200	4.16320900
H	0	5.63231700	-4.70478800	3.86724500
Si	0	-1.77257300	1.73703400	5.13275600
Cl	0	-0.33420100	0.23110800	5.05991100
Cl	0	-3.37045300	0.26118000	4.47742100
Cl	0	-2.86546100	2.09221300	6.85473200
Cl	0	-0.37345900	3.31973300	5.53918300

TS2$^{A\text{-}Si}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000

Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76010000	0.00000000	0.74280000
Si	-1	-5.76010000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000

H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000

H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.04884000	5.75414200	1.96152600
Si	0	-5.14546000	1.93956800	1.95736700
Si	0	-5.05361100	-1.92824100	1.96880100
Si	0	-5.03468600	-5.74654100	1.96529000
Si	0	-2.63051700	5.74475600	1.95282100
Si	0	-2.71173100	1.94830000	1.83606100
Si	0	-2.58522600	-1.96059200	1.96340600
Si	0	-2.61192700	-5.75480000	1.94766600
Si	0	2.60768100	5.75111600	1.95630400
Si	0	2.64928900	1.92276800	1.93541500
Si	0	2.59747600	-1.92119600	1.96346200
Si	0	2.59286800	-5.75491900	1.95271100
Si	0	5.03537000	5.76749500	1.96927500
Si	0	5.06579500	1.90800900	1.92730900
Si	0	5.05688400	-1.93225300	1.95101400
Si	0	5.02350400	-5.74527400	1.96442500
O	0	-5.36555900	5.63566400	3.61160500
O	0	-5.68185500	2.17511800	3.52450600
O	0	-5.59608300	-1.87409200	3.55559700
O	0	-5.36335600	-5.51904300	3.59899600
O	0	-2.28139900	5.54334300	3.58091500
O	0	-2.17642600	2.42801600	3.56507400
O	0	-1.91902500	-2.23662700	3.47665200
O	0	-2.37555100	-5.74773100	3.61284200
O	0	2.36248700	5.71718700	3.61095700
O	0	2.52396900	1.91918300	3.60155300
O	0	2.14230800	-1.95784800	3.57669900
O	0	2.17837200	-5.72678900	3.57776900
O	0	5.36297300	5.72208200	3.60440000
O	0	5.39283600	1.77778200	3.56107100
O	0	5.61063300	-2.15162200	3.52210400

O	0	5.33454700	-5.59559000	3.61407800
H	0	-5.74128800	4.79307800	3.90025500
H	0	-5.58323500	1.43167000	4.13417000
H	0	-5.70569200	-2.74185800	3.96844500
H	0	-4.58501600	-5.70399800	4.14736800
H	0	-3.04311700	5.72926800	4.15097100
H	0	-1.58959800	3.25541100	3.57377300
H	0	-2.25748100	-1.70440300	4.20681100
H	0	-1.50641400	-5.49769400	3.94746400
H	0	1.55490900	5.31067400	3.96293500
H	0	1.73893000	2.32425500	4.01242200
H	0	1.27158500	-2.33451000	3.75447100
H	0	2.96286900	-5.66372600	4.14318600
H	0	4.55447700	5.65511200	4.13547400
H	0	4.59616700	1.96675400	4.08436200
H	0	5.40800000	-1.43587000	4.13833000
H	0	5.66563300	-4.72555700	3.87890000
Si	0	-1.74063100	1.54361500	4.97156900
Cl	0	-0.17908900	0.27382000	4.73379400
Cl	0	-3.39908900	0.24573500	4.84427300
Cl	0	-2.05410000	2.41002300	6.76881200
Cl	0	0.08801300	3.55307300	4.58369200

Im3$^{A\text{-}Si}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000100	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260100
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000

Si	-1	-3.84009900	3.84010100	-0.61490100
Si	-1	-3.84009800	-0.00000100	-0.61490200
Si	-1	-3.84010000	-3.84009900	-0.61489900
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	-0.00000100	7.68020100	-0.61489800
Si	-1	-0.00000100	3.84009900	-0.61489900
Si	-1	0.00000100	-0.00000200	-0.61489900
Si	-1	0.00000000	-3.84009900	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68019900	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61489900
Si	-1	3.84010000	-0.00000100	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010100	7.68020300	0.74280000
Si	-1	-5.76009900	3.84010000	0.74280000
Si	-1	-5.76010400	0.00000100	0.74280000
Si	-1	-5.76009800	-3.84010100	0.74279900
Si	-1	-5.76010000	-7.68019900	0.74280100
Si	-1	-1.91999600	7.68020100	0.74279800
Si	-1	-1.92000600	3.84009700	0.74280700
Si	-1	-1.91999900	0.00000000	0.74279800
Si	-1	-1.91999900	-3.84010300	0.74279900
Si	-1	-1.92000000	-7.68019900	0.74280000
Si	-1	1.92000000	7.68020100	0.74279700
Si	-1	1.92000300	3.84010200	0.74280000
Si	-1	1.92000000	0.00000200	0.74280100
Si	-1	1.92000000	-3.84010100	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010100	7.68020200	0.74279900
Si	-1	5.76010000	3.84009900	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000

H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40189900	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980100
H	-1	-7.05960000	3.84789900	0.03190000
H	-1	-7.05809900	0.00000000	0.02889900
H	-1	-7.05950100	-3.84759900	0.03180100
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150200	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880100
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87619900	8.93250000	1.53080100

H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.04487400	5.74291300	1.96066700
Si	0	-5.08776900	1.94102900	1.93893800
Si	0	-5.04416900	-1.93841600	1.94776300
Si	0	-5.03243000	-5.74005200	1.96601900
Si	0	-2.63379100	5.75882900	1.91091300
Si	0	-2.64592800	1.90746700	1.91364000
Si	0	-2.60560400	-1.91841000	1.95070600
Si	0	-2.60835500	-5.75471200	1.94590900
Si	0	2.62850200	5.75708700	1.94874500
Si	0	2.61127600	1.91879800	1.94668300
Si	0	2.62281200	-1.91564300	1.93329400
Si	0	2.59243000	-5.75818900	1.95397300
Si	0	5.04401700	5.74216400	1.95367200
Si	0	5.03674700	1.94043700	1.92673700
Si	0	5.04504700	-1.94676600	1.93488100
Si	0	5.02258200	-5.74387900	1.96544700
O	0	-5.28535600	5.56806500	3.62291300
O	0	-5.62814800	2.20207300	3.51115300
O	0	-5.44662300	-2.02174200	3.58110500
O	0	-5.36756000	-5.47781200	3.59717200
O	0	-2.29741300	5.72732500	3.59265900
O	0	-2.22375700	1.81736400	3.53909500
O	0	-2.14502500	-1.91415000	3.56341300
O	0	-2.36438400	-5.74323900	3.61127600
O	0	2.47097300	5.78500000	3.61771000
O	0	2.28571900	1.90282200	3.58842600
O	0	2.40241700	-1.88028900	3.60132400
O	0	2.17309900	-5.76224600	3.57682300
O	0	5.36515600	5.49382400	3.58717000
O	0	5.35496600	2.05658300	3.57952200
O	0	5.39811900	-2.17215500	3.56503400
O	0	5.34280600	-5.57805300	3.61183500

H	0	-5.64902800	4.71122900	3.89083900
H	0	-5.60513900	1.45226000	4.12117400
H	0	-5.69884500	-2.91039500	3.87205900
H	0	-4.60854300	-5.69610500	4.15978700
H	0	-3.11082500	5.62397500	4.11977600
H	0	-1.13238900	4.84806600	3.95456100
H	0	-2.89284800	-1.85492400	4.17531500
H	0	-1.46581700	-5.61063500	3.93653700
H	0	1.67597500	5.37675400	3.99560800
H	0	3.10067000	1.94540900	4.11201300
H	0	1.53544200	-1.62440500	3.93908800
H	0	2.94952500	-5.66848600	4.14810700
H	0	4.56916800	5.66815300	4.11688400
H	0	5.68038700	2.92620800	3.85412500
H	0	4.67590400	-1.86945200	4.13679500
H	0	5.64274300	-4.69205200	3.86186200
Si	0	-2.41989800	1.59850200	5.10480800
Cl	0	-0.72604000	0.94537300	5.99926100
Cl	0	-3.88878700	0.18095800	5.41988200
Cl	0	-3.07670800	3.31620300	6.00061000
Cl	0	-0.06046000	4.00701300	4.05408600

P1[A-Si]

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260100
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97259900
Si	-1	0.00000000	-1.92000100	-1.97259900
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84009700	-0.61490100

Si	-1	-3.84009900	-0.00000100	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	-0.00000200	3.84009800	-0.61490100
Si	-1	-0.00000100	0.00000200	-0.61490400
Si	-1	-0.00000100	-3.84010000	-0.61490100
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010100	7.68020000	0.74280100
Si	-1	-5.76009800	3.84009600	0.74279500
Si	-1	-5.76009500	0.00000300	0.74278900
Si	-1	-5.76009900	-3.84009900	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000200	7.68019700	0.74279800
Si	-1	-1.91999500	3.84011100	0.74280600
Si	-1	-1.92000600	-0.00000700	0.74280500
Si	-1	-1.91999700	-3.84010000	0.74280100
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280100
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000

H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87799900	8.93300000	1.52980000
H	-1	-7.05960200	3.84790100	0.03190300
H	-1	-7.05810300	-0.00000100	0.02890600
H	-1	-7.05950000	-3.84760100	0.03180100
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90149900	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000

H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.02571000	5.74531500	1.97074600
Si	0	-5.08283000	1.94521700	1.94742500
Si	0	-5.04127600	-1.93898800	1.94575400
Si	0	-5.03312500	-5.73990600	1.96530000
Si	0	-2.59483500	5.75674500	1.96044400
Si	0	-2.62613300	1.91813600	1.91820700
Si	0	-2.60472000	-1.91802300	1.94393300
Si	0	-2.60881200	-5.75442600	1.94532000
Si	0	2.60735500	5.75362000	1.94549800
Si	0	2.61473300	1.91931100	1.94259400
Si	0	2.62317200	-1.91604500	1.93288600
Si	0	2.59268100	-5.75812200	1.95413200
Si	0	5.03186400	5.74038800	1.96511000
Si	0	5.03912500	1.93843200	1.92816600
Si	0	5.04536900	-1.94695100	1.93570400
Si	0	5.02266900	-5.74421700	1.96554200
O	0	-5.34874600	5.58819600	3.61591800
O	0	-5.64268300	2.22171300	3.50958900
O	0	-5.42046900	-2.03699900	3.58522800
O	0	-5.37016000	-5.47933900	3.59657100
O	0	-2.16895400	5.74011200	3.57966000
O	0	-2.10242200	1.92770800	3.52781100
O	0	-2.14619700	-1.89805400	3.55849500
O	0	-2.36472000	-5.74350800	3.61130200
O	0	2.36316300	5.74103900	3.61043200
O	0	2.26959900	1.92798500	3.58076500
O	0	2.40019300	-1.88022700	3.60068700
O	0	2.17391100	-5.76126400	3.57735600
O	0	5.36583800	5.48556300	3.59719200
O	0	5.35769000	2.04914000	3.58099200
O	0	5.39954900	-2.17069500	3.56582900
O	0	5.34273000	-5.57924000	3.61214400
H	0	-5.68766100	4.71973200	3.87592800

H	0	-5.57117600	1.49383000	4.14098400
H	0	-5.70306200	-2.92023000	3.86445500
H	0	-4.61423200	-5.70365900	4.16080700
H	0	-2.93662300	5.64744500	4.16280700
H	0	-2.89910900	-1.94241600	4.16586700
H	0	-1.46046900	-5.65485700	3.93588200
H	0	1.47695300	5.54866000	3.93960000
H	0	3.07880500	1.93540600	4.11437300
H	0	1.52210800	-1.65736100	3.93319900
H	0	2.95116700	-5.67160200	4.14822100
H	0	4.59962300	5.68863000	4.15588900
H	0	5.67712500	2.91944200	3.85987500
H	0	4.67661900	-1.87102900	4.13814700
H	0	5.64537200	-4.69438700	3.86266500
Si	0	-2.22304600	1.49456400	5.06060200
Cl	0	-0.54863400	0.54622000	5.70494900
Cl	0	-3.82392000	0.22107300	5.33005400
Cl	0	-2.54989300	3.13448300	6.22511000

Im1$^{A\text{-}Al}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000

Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76010000	0.00000000	0.74280000
Si	-1	-5.76010000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000

H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000

H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.02897000	5.75683200	1.95845500
Si	0	-5.07809400	1.92417900	1.95043800
Si	0	-5.11462900	-1.90489300	1.96280000
Si	0	-5.04551000	-5.76311000	1.97630500
Si	0	-2.60305100	5.75017100	1.95402700
Si	0	-2.62852400	1.88404800	1.94164000
Si	0	-2.66773300	-1.88061600	1.88830700
Si	0	-2.62129500	-5.77548600	1.95375900
Si	0	2.61039100	5.75345400	1.94428200
Si	0	2.61132500	1.92421200	1.94318700
Si	0	2.62669700	-1.92176100	1.93851800
Si	0	2.59887300	-5.75596700	1.95487400
Si	0	5.03406400	5.74082500	1.96375000
Si	0	5.04004700	1.93532200	1.93169100
Si	0	5.04768500	-1.94448400	1.93113600
Si	0	5.02655800	-5.74429300	1.96046500
O	0	-5.32212500	5.66553800	3.61719100
O	0	-5.61319500	2.02713100	3.53895000
O	0	-5.63065500	-1.66170300	3.53143500
O	0	-5.39759400	-5.65264600	3.60304500
O	0	-2.22812300	5.64042000	3.58751800
O	0	-2.10293700	1.44107700	3.50105000
O	0	-2.13222400	-1.43584000	3.54608900
O	0	-2.37568200	-5.86403400	3.60330000
O	0	2.36869100	5.74567800	3.60990100
O	0	2.23673300	1.99877400	3.57183800
O	0	2.43689300	-1.91460600	3.60538400
O	0	2.21577900	-5.72582900	3.58402900
O	0	5.36321600	5.48999400	3.59644700
O	0	5.37910100	2.02328600	3.57873600
O	0	5.39151700	-2.17671300	3.56106200
O	0	5.34369500	-5.58413000	3.60804200
H	0	-5.77973900	4.87315900	3.92401300
H	0	-5.69882200	1.18177500	3.99996500
H	0	-5.39156500	-2.34173800	4.17966200
H	0	-4.60337500	-5.64986400	4.16173800

H	0	-3.01249600	5.78135200	4.13941100
H	0	-2.15330100	2.08085700	4.22198300
H	0	-2.04108200	-0.45607800	3.66272300
H	0	-1.49679500	-5.68534700	3.96446500
H	0	1.50472300	5.47854800	3.94420800
H	0	3.00796100	1.83271500	4.13330000
H	0	1.67710800	-2.37800700	3.98658700
H	0	3.00660500	-5.71098700	4.14379100
H	0	4.59257500	5.68589400	4.15169000
H	0	5.65253800	2.90268700	3.87668600
H	0	4.63460800	-1.93741500	4.11969500
H	0	5.63606700	-4.69691600	3.86312000
Al	0	-1.80627000	-2.42796500	5.06255500
Cl	0	-0.18760600	-3.71755700	4.48680900
Cl	0	-3.62958900	-3.47615500	5.41664300
Cl	0	-1.29558900	-0.97502300	6.50280700

TS1$^{A\text{-}Al}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000

Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76010000	0.00000000	0.74280000
Si	-1	-5.76010000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000

H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000

Si	0	-5.02468900	5.74484400	1.96965200
Si	0	-5.05831700	1.94656200	1.94115900
Si	0	-5.09128200	-1.90614500	1.97078300
Si	0	-5.10759800	-5.77753200	2.01635100
Si	0	-2.59367900	5.75946600	1.95699400
Si	0	-2.63672100	1.91844900	1.95440500
Si	0	-2.63338600	-1.95547600	1.87961100
Si	0	-2.60820800	-5.69745900	1.95545100
Si	0	2.60844000	5.75475100	1.94569900
Si	0	2.61330700	1.91814700	1.94005400
Si	0	2.62202000	-1.91937800	1.93785500
Si	0	2.54044800	-5.75904200	1.97674900
Si	0	5.03321200	5.74108600	1.96545900
Si	0	5.03831200	1.93926300	1.93151300
Si	0	5.04787100	-1.94760000	1.93375900
Si	0	5.03341400	-5.75093600	2.00600700
O	0	-5.35000800	5.58323900	3.61302200
O	0	-5.43277000	2.17247900	3.56010500
O	0	-5.59477700	-1.72619300	3.54297000
O	0	-5.69841900	-5.94549300	3.55446600
O	0	-2.16288300	5.75965000	3.57512500
O	0	-2.45860900	1.85308100	3.61868200
O	0	-1.94733300	-2.28389600	3.44683500
O	0	-1.85126800	-5.30182600	3.54845300
O	0	2.36397000	5.74129300	3.61054600
O	0	2.23707500	1.88667500	3.57199400
O	0	2.40452600	-1.95813700	3.60813400
O	0	1.74742300	-5.84658700	3.45727300
O	0	5.37182000	5.48825800	3.59609000
O	0	5.34942600	2.04887100	3.58436900
O	0	5.40147400	-2.17056400	3.56193600
O	0	5.57505000	-5.64404600	3.58255300
H	0	-5.64679000	4.69896300	3.87280400
H	0	-4.76739700	1.79442200	4.15624100
H	0	-5.18990000	-2.26193600	4.23926900
H	0	-5.36221500	-5.35702900	4.24362200
H	0	-2.92979400	5.65869100	4.15761200
H	0	-1.64158200	1.56093400	4.04097600

H	0	-1.91892300	-1.50498600	4.22745400
H	0	-0.97680700	-5.71566500	3.68410300
H	0	1.46414300	5.62501800	3.93855200
H	0	3.02988500	1.95166500	4.12572700
H	0	1.56618700	-1.67899200	3.99686300
H	0	1.91164000	-5.13344600	4.08905600
H	0	4.61264100	5.70072400	4.16053500
H	0	5.69646200	2.90757600	3.86542800
H	0	4.68486300	-1.86856100	4.14059100
H	0	5.69612600	-4.73717300	3.89734600
Al	0	-1.92492200	-3.67599400	4.63070100
Cl	0	-0.09168800	-4.10162500	5.60699700
Cl	0	-3.90459600	-3.96789600	5.40153500
Cl	0	-1.82952800	-1.05926700	5.81835700

Im2$^{A\text{-}Al}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010100	-1.97259700
Si	-1	-3.84010100	1.91999600	-1.97260700
Si	-1	-3.84009700	-1.91997700	-1.97258900
Si	-1	-3.84010600	-5.76009700	-1.97259100
Si	-1	0.00000100	5.76010100	-1.97259900
Si	-1	0.00000100	1.92000200	-1.97259600
Si	-1	0.00000100	-1.92000300	-1.97259700
Si	-1	-0.00001000	-5.76010300	-1.97261700
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020300	-0.61490100
Si	-1	-3.84010500	3.84011200	-0.61491100
Si	-1	-3.84013100	0.00004800	-0.61489400
Si	-1	-3.84006600	-3.84012500	-0.61491700
Si	-1	-3.84009900	-7.68022900	-0.61493500
Si	-1	0.00000200	7.68020000	-0.61489800
Si	-1	-0.00000200	3.84011000	-0.61490300
Si	-1	-0.00002500	0.00001800	-0.61493700
Si	-1	0.00004900	-3.84009300	-0.61483100

Si	-1	0.00003500	-7.68025100	-0.61485300
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84009900	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84009900	-0.61489800
Si	-1	3.84009900	-7.68019900	-0.61490100
Si	-1	-5.76011000	7.68020900	0.74279300
Si	-1	-5.76009200	3.84009400	0.74280700
Si	-1	-5.75997100	-0.00006900	0.74286600
Si	-1	-5.76008500	-3.84023000	0.74265100
Si	-1	-5.76007400	-7.68016400	0.74292200
Si	-1	-1.92000900	7.68020500	0.74279600
Si	-1	-1.91998500	3.84010700	0.74278100
Si	-1	-1.92004000	-0.00013300	0.74289700
Si	-1	-1.92000800	-3.84024700	0.74264200
Si	-1	-1.92016900	-7.67980400	0.74280200
Si	-1	1.92000100	7.68019900	0.74279900
Si	-1	1.92000200	3.84010100	0.74279900
Si	-1	1.91999700	-0.00000600	0.74280000
Si	-1	1.92000400	-3.84011000	0.74280000
Si	-1	1.91999300	-7.68017700	0.74279600
Si	-1	5.76010100	7.68020000	0.74280000
Si	-1	5.76010100	3.84010000	0.74280000
Si	-1	5.76009800	-0.00000100	0.74280200
Si	-1	5.76010000	-3.84009900	0.74280400
Si	-1	5.76010000	-7.68019700	0.74280600
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000

H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82399800	8.85870000	-1.53420000
H	-1	-3.82401100	-8.85870600	-1.53419200
H	-1	0.00000100	8.92610100	-1.42909800
H	-1	0.00000600	-8.92611000	-1.42908400
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400100	-8.85870100	-1.53419900
H	-1	-7.00579900	7.40190300	-0.01410200
H	-1	-5.87800100	8.93300100	1.52979800
H	-1	-7.05959900	3.84791100	0.03189800
H	-1	-7.05811400	0.00001500	0.02892600
H	-1	-7.05951600	-3.84758200	0.03182900
H	-1	-5.87620200	-8.93251400	1.53077700
H	-1	-7.00649200	-7.40339600	-0.01331200
H	-1	-1.90150200	8.88670000	1.61890000
H	-1	-1.90147900	-8.88671400	1.61878100
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150900	-8.88670300	1.61889700
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	-0.00000100	0.02890000
H	-1	7.05959900	-3.84790100	0.03189800
H	-1	7.00579800	-7.40189900	-0.01410200
H	-1	5.87799900	-8.93300000	1.52979900
Si	0	-5.02362900	5.74004000	1.97083700
Si	0	-5.05212400	1.95970400	1.97014200

Si	0	-5.05532500	-1.94625100	1.94188800
Si	0	-5.07040900	-5.72591500	2.01678800
Si	0	-2.59126500	5.75852200	1.95502200
Si	0	-2.59579800	1.93308300	1.97397000
Si	0	-2.59118400	-1.96233500	1.99188000
Si	0	-2.56535900	-5.71262100	1.92993800
Si	0	2.60917600	5.75537900	1.94509100
Si	0	2.60763700	1.92099300	1.93890600
Si	0	2.62305400	-1.92116800	1.93872900
Si	0	2.52168000	-5.75803500	1.97759500
Si	0	5.03329700	5.74030500	1.96502600
Si	0	5.03604300	1.93884400	1.93591600
Si	0	5.04864200	-1.94635300	1.93453900
Si	0	5.02700800	-5.75045800	2.01154900
O	0	-5.35177900	5.54658300	3.60978000
O	0	-5.60145600	2.27852100	3.52098500
O	0	-5.63005600	-2.12929600	3.53855200
O	0	-5.62933800	-5.40553100	3.56433000
O	0	-2.15683400	5.77009600	3.57362800
O	0	-2.16340100	2.01130900	3.58397300
O	0	-2.07148600	-2.35092300	3.51181500
O	0	-1.74984300	-5.39445500	3.51180200
O	0	2.36753200	5.75293500	3.61110600
O	0	2.19881700	1.92823500	3.56544300
O	0	2.42046700	-1.97398600	3.60829300
O	0	1.66913800	-5.84511600	3.43376100
O	0	5.36955700	5.48646000	3.59676000
O	0	5.35824200	2.04478600	3.58645900
O	0	5.40394100	-2.17685800	3.56216700
O	0	5.57177100	-5.64089600	3.58695400
H	0	-5.63383500	4.64766100	3.84105400
H	0	-5.23594100	1.69870700	4.20893800
H	0	-5.70428800	-3.05465600	3.82990600
H	0	-5.13025500	-5.72021100	4.32961400
H	0	-2.91816600	5.61965400	4.15288600
H	0	-1.22262900	2.07207600	3.78907000
H	0	-4.81644200	-1.13706300	4.54507600
H	0	-0.83811800	-5.74984000	3.56128600

H	0	1.46338200	5.68402700	3.94026800
H	0	2.98050100	1.91957900	4.13744600
H	0	1.53291200	-1.97839900	3.99182300
H	0	1.82902200	-5.14233700	4.07936900
H	0	4.61015300	5.70461900	4.15881300
H	0	5.67523700	2.91479900	3.86875800
H	0	4.68037100	-1.89088800	4.14039000
H	0	5.69664400	-4.73226200	3.89568100
Al	0	-1.87961900	-3.74830600	4.50142300
Cl	0	0.04696600	-3.76096800	5.43413400
Cl	0	-3.57201200	-4.16491800	5.72514600
Cl	0	-4.03538700	-0.14641200	4.97408300

P1$^{\text{A-Al}}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.91999900	-1.97260000
Si	-1	-3.84009700	-1.92000200	-1.97259800
Si	-1	-3.84009900	-5.76009900	-1.97260100
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.91999900	-1.97260100
Si	-1	0.00000000	-1.92000200	-1.97260100
Si	-1	-0.00000300	-5.76009900	-1.97259700
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84009900	-1.92000200	-1.97260200
Si	-1	3.84010200	-5.76010100	-1.97259600
Si	-1	-3.84010000	7.68019900	-0.61490000
Si	-1	-3.84010000	3.84009900	-0.61490000
Si	-1	-3.84010100	0.00000200	-0.61490600
Si	-1	-3.84010900	-3.84009100	-0.61489400
Si	-1	-3.84009800	-7.68020100	-0.61490000
Si	-1	0.00000000	7.68019900	-0.61490000
Si	-1	0.00000100	3.84009800	-0.61490000
Si	-1	-0.00000300	0.00000200	-0.61490300
Si	-1	0.00000400	-3.84010200	-0.61490600
Si	-1	0.00000500	-7.68019200	-0.61490200
Si	-1	3.84010000	7.68020000	-0.61490000

Si	-1	3.84010000	3.84009900	-0.61490000
Si	-1	3.84009900	-0.00000200	-0.61490000
Si	-1	3.84009800	-3.84010200	-0.61490700
Si	-1	3.84009600	-7.68019600	-0.61490200
Si	-1	-5.76009900	7.68019900	0.74280100
Si	-1	-5.76010200	3.84010300	0.74279800
Si	-1	-5.76007900	0.00000800	0.74278600
Si	-1	-5.76014000	-3.84014300	0.74281100
Si	-1	-5.76009200	-7.68016300	0.74277900
Si	-1	-1.92000000	7.68019900	0.74280000
Si	-1	-1.92000300	3.84010300	0.74279700
Si	-1	-1.92000300	0.00002800	0.74281000
Si	-1	-1.91998800	-3.84010400	0.74280200
Si	-1	-1.91997900	-7.68024600	0.74280400
Si	-1	1.92000000	7.68019900	0.74280000
Si	-1	1.92000000	3.84009800	0.74279900
Si	-1	1.91999600	0.00000400	0.74279900
Si	-1	1.92001600	-3.84004900	0.74281200
Si	-1	1.91997800	-7.68026100	0.74280900
Si	-1	5.76009900	7.68019900	0.74280000
Si	-1	5.76010000	3.84009900	0.74280000
Si	-1	5.76010200	0.00000100	0.74279900
Si	-1	5.76010600	-3.84008600	0.74279800
Si	-1	5.76008700	-7.68020900	0.74280400
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000

H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82399700	-8.85870100	-1.53419800
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	-0.00000100	-8.92609300	-1.42911000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85869700	-1.53420300
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87799900	8.93300000	1.52980000
H	-1	-7.05960100	3.84789900	0.03190200
H	-1	-7.05809800	-0.00000100	0.02889600
H	-1	-7.05950500	-3.84758900	0.03180800
H	-1	-5.87619900	-8.93249800	1.53080300
H	-1	-7.00650400	-7.40340700	-0.01329600
H	-1	-1.90149900	8.88670000	1.61890100
H	-1	-1.90150300	-8.88669900	1.61880100
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150600	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84759900	0.03180000
H	-1	7.05809900	-0.00000100	0.02889900
H	-1	7.05960100	-3.84790100	0.03190200
H	-1	7.00579800	-7.40189900	-0.01410300
H	-1	5.87801000	-8.93299800	1.52980200
Si	0	-5.02400300	5.74389000	1.96634500
Si	0	-5.05440800	1.94515100	1.93912500
Si	0	-5.05566700	-1.90782700	1.96434900
Si	0	-5.09982700	-5.77335800	2.01692800

Si	0	-2.59443400	5.75731600	1.95434200
Si	0	-2.62925700	1.92140900	1.93731900
Si	0	-2.59300500	-1.95594300	1.97354000
Si	0	-2.59533900	-5.71185500	1.92498100
Si	0	2.60978300	5.75510600	1.94455000
Si	0	2.61132100	1.91893400	1.93936900
Si	0	2.62258900	-1.92274400	1.93704100
Si	0	2.52785200	-5.75613700	1.97800000
Si	0	5.03391700	5.74048100	1.96502200
Si	0	5.03693400	1.93917100	1.93223500
Si	0	5.04855100	-1.94671800	1.93523000
Si	0	5.02849900	-5.75022800	2.01024900
O	0	-5.34230500	5.57664100	3.61248500
O	0	-5.43364600	2.19397600	3.55852300
O	0	-5.57194400	-1.77873200	3.54584400
O	0	-5.66164500	-5.92484500	3.56873500
O	0	-2.17843200	5.74663900	3.57882000
O	0	-2.39385300	1.89779100	3.60201500
O	0	-2.04645500	-2.27939400	3.50946900
O	0	-1.78787400	-5.36236300	3.51703500
O	0	2.36703500	5.75089400	3.61087100
O	0	2.23114800	1.91322000	3.57296000
O	0	2.40712000	-1.98017900	3.60723300
O	0	1.69851400	-5.82412500	3.44857300
O	0	5.37107000	5.48758900	3.59667600
O	0	5.34935900	2.05191600	3.58550300
O	0	5.40618700	-2.17492800	3.56310800
O	0	5.56894800	-5.63699300	3.58752100
H	0	-5.63639700	4.68851900	3.86311900
H	0	-4.78194000	1.80753500	4.16157300
H	0	-5.08787100	-2.28485600	4.21338500
H	0	-5.34153500	-5.30873900	4.24160400
H	0	-2.96011600	5.67360400	4.14643700
H	0	-1.48936000	1.90069200	3.93661100
H	0	-0.88921600	-5.73983600	3.59828500
H	0	1.46279800	5.67520000	3.93803700
H	0	3.02864300	1.94865900	4.12272700
H	0	1.51604300	-1.92988700	3.97704800

H	0	1.90510700	-5.13537600	4.09485700
H	0	4.61186300	5.70488500	4.15921500
H	0	5.68598000	2.91596200	3.86323500
H	0	4.68857400	-1.87952600	4.14353800
H	0	5.70269200	-4.72792100	3.89099700
Al	0	-1.92885100	-3.71445400	4.46499100
Cl	0	-0.11252500	-3.78290100	5.57433400
Cl	0	-3.79001400	-3.99917200	5.50494900

Im1$^{B\text{-}OiPr}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	-0.00000100	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490100
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010100	3.84009900	-0.61490000
Si	-1	3.84010100	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010100	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000

Si	-1	-5.76010000	7.68019900	0.74280000
Si	-1	-5.76009700	3.84020000	0.74279900
Si	-1	-5.76010300	0.00000000	0.74289900
Si	-1	-5.76009900	-3.84020100	0.74270100
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280100
Si	-1	-1.91989700	3.84009800	0.74280100
Si	-1	-1.92010100	-0.00000100	0.74290000
Si	-1	-1.91999900	-3.84009900	0.74280100
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000200	7.68019800	0.74280000
Si	-1	1.92000000	3.84010100	0.74280000
Si	-1	1.92000100	0.00000300	0.74279800
Si	-1	1.92000100	-3.84009900	0.74279900
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68019900	0.74280100
Si	-1	5.76009700	3.84010000	0.74279900
Si	-1	5.76009800	0.00000200	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000

H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02880000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950100	3.84760000	0.03180100
H	-1	7.05810000	0.00000000	0.02890100
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00520900	5.77779800	2.04529900
Si	0	-5.07083700	1.89630900	1.89798000
Si	0	-4.96292100	-1.92830100	1.99883300
Si	0	-5.04126900	-5.75550300	1.94039400
Si	0	-2.42858900	5.74752400	2.02930700
Si	0	-2.62938800	1.91780100	1.89012600
Si	0	-2.45504300	-1.89775300	2.01972100
Si	0	-2.60622300	-5.74629300	1.93752900

Si	0	2.38852100	5.76082700	1.94457800
Si	0	2.69203600	2.00791500	1.98036700
Si	0	2.37091500	-1.92988900	1.97498200
Si	0	2.60779500	-5.74237400	1.94035100
Si	0	4.83151600	5.64723600	1.98477200
Si	0	5.11363400	1.91342100	1.91118400
Si	0	4.91681900	-1.94661500	2.00460600
Si	0	5.04260900	-5.75244000	1.94011800
O	0	-5.63157200	5.86856200	3.58156500
O	0	-5.32936800	1.73488300	3.53507700
O	0	-5.30696900	-2.02863900	3.64632200
O	0	-5.25455900	-5.63377500	3.60865700
O	0	-1.45546700	5.68855100	3.39345900
O	0	-2.40299000	1.87287800	3.62962400
O	0	-1.67685000	-1.71790200	3.47454200
O	0	-2.39701100	-5.64519000	3.60365000
O	0	1.64598000	5.81877100	3.42599800
O	0	1.38320000	-1.93775200	3.28351800
O	0	2.40535500	-5.62074000	3.60370800
O	0	5.23296800	-2.08872400	3.64928300
O	0	5.25721600	-5.60385600	3.60392000
H	0	-5.37326900	5.19836200	4.22941400
H	0	-6.22067500	-2.21218100	3.89264500
Al	0	-4.00320200	1.90473900	4.60825000
Al	0	-3.82103700	-5.43209500	4.53599500
Cl	0	-4.36615000	3.60930800	5.83171300
Cl	0	-3.87527800	-5.08986200	6.57930500
Al	0	-0.07841400	-1.81012200	4.21211300
Al	0	0.06635900	6.14941300	4.05255000
Cl	0	-0.01960400	-3.23488800	5.79556800
Cl	0	-0.00862200	7.90267200	5.22385000
Al	0	3.82753800	-5.32357200	4.52032800
Cl	0	3.87661100	-4.83416900	6.53078900
H	0	6.14232400	-2.24284900	3.92911200
Al	0	-1.47278400	1.05259400	5.00005300
O	0	-3.18304600	0.55827900	5.51488000
O	0	-0.96816200	2.30273100	6.05027700
O	0	-0.06383100	-0.07720200	4.94963200

C	0	-3.64851900	-0.19891200	6.67084200
C	0	-2.83602400	-1.47201300	6.73199500
C	0	-1.01908400	3.70301600	6.11641800
C	0	-1.31937800	4.12899500	7.54452800
C	0	1.10630500	0.38207000	5.78302300
C	0	0.80535300	0.07606000	7.23722000
H	0	-4.69611400	-0.43614900	6.45701300
C	0	-3.53034500	0.65752800	7.91861400
H	0	-2.89015400	-2.00575600	5.77960500
H	0	-3.20299900	-2.12945500	7.52333700
H	0	-1.78544900	-1.24691300	6.95073500
H	0	-1.79792500	4.09557500	5.44994100
C	0	0.32088700	4.25413800	5.64178300
H	0	-2.27798700	3.71127700	7.85916200
H	0	-1.37411000	5.21910300	7.62703600
H	0	-0.53610000	3.75939200	8.21407700
H	0	1.15616300	1.45776600	5.61407000
C	0	2.41935000	-0.22719800	5.33232900
H	0	0.72674100	-1.00352600	7.39423100
H	0	-0.11331200	0.57124800	7.56100600
H	0	1.62243500	0.45877000	7.85554800
H	0	-3.83866100	0.07875100	8.79298200
H	0	-4.15510100	1.55201100	7.85538400
H	0	-2.49150100	0.97480700	8.05790600
H	0	2.63150700	0.00000900	4.28647000
H	0	2.46797600	-1.30801000	5.48707400
H	0	3.20046200	0.24001900	5.94162200
H	0	0.53770100	3.97651600	4.59937200
H	0	1.16369000	3.85658100	6.21801300
H	0	0.37870800	5.34026000	5.86617500
O	0	2.63609000	2.55989000	3.57435300
O	0	4.82415700	4.94259200	3.67906200
O	0	5.41320200	2.14498400	3.52895800
Al	0	4.17046400	3.13618200	4.24601000
Cl	0	4.04146800	3.54166100	6.32346400
H	0	4.60390800	5.56798200	4.38883200

TS1$^{B\text{-}OiPr}$

Atom	Fix/Relax	X	Y	Z
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84020000	0.74280000
Si	-1	-5.76010000	0.00000000	0.74290000
Si	-1	-5.76010000	-3.84020000	0.74270000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.91990000	3.84010000	0.74280000
Si	-1	-1.92010000	0.00000000	0.74290000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68020000	0.74280000

Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000

H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02880000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00093100	5.77275000	2.04655500
Si	0	-5.07194800	1.90306500	1.90846100
Si	0	-4.96631900	-1.93362000	1.99075500
Si	0	-5.03625500	-5.75335700	1.93960200
Si	0	-2.42384700	5.74569900	2.02794300
Si	0	-2.64213500	1.94897800	1.87918000
Si	0	-2.43307600	-1.94630600	2.02445000
Si	0	-2.59960800	-5.74687600	1.93652300
Si	0	2.39173900	5.76389200	1.93923400
Si	0	2.68335400	2.00283200	1.99431800
Si	0	2.40209500	-1.92596400	1.98752200
Si	0	2.60379100	-5.74274000	1.94019700
Si	0	4.83597700	5.65784600	1.96870400
Si	0	5.11044900	1.91212900	1.90318500
Si	0	4.92783100	-1.94196600	1.99284300
Si	0	5.04003300	-5.75156000	1.94005600
O	0	-5.61338700	5.85184700	3.59080500
O	0	-5.30655600	1.81617000	3.55577700

O	0	-5.39902400	-2.03752200	3.61493100
O	0	-5.24715800	-5.63451300	3.60880300
O	0	-1.44400100	5.70170700	3.39089500
O	0	-2.44163400	2.15836200	3.59632500
O	0	-1.59181900	-2.08174300	3.43046300
O	0	-2.38716100	-5.68453100	3.60339000
O	0	1.66554900	5.83320900	3.42529400
O	0	1.55644400	-1.93974800	3.39996300
O	0	2.40164500	-5.61795700	3.60631800
O	0	5.25044700	-2.05240800	3.64687900
O	0	5.25959600	-5.58399400	3.60413400
H	0	-5.36019000	5.17514200	4.23359600
H	0	-6.31551200	-2.26565900	3.80704600
Al	0	-3.96915400	1.99031700	4.62546200
Al	0	-3.80958800	-5.46150300	4.53575000
Cl	0	-4.34654900	3.55001900	6.02534000
Cl	0	-3.84077600	-5.19047600	6.58929700
Al	0	0.07667700	6.18425000	4.03059600
Cl	0	0.02164500	7.96848600	5.15560000
Al	0	3.82532500	-5.29282200	4.50778600
Cl	0	3.87209000	-4.71705500	6.49824000
H	0	6.14796100	-2.28747700	3.90968600
O	0	-0.67303400	2.25653600	5.97804900
C	0	-0.83623100	3.63918700	6.17392400
C	0	-1.03303500	3.95177700	7.64891100
H	0	-1.70366100	4.01945600	5.61517600
C	0	0.40250300	4.32547300	5.61758000
H	0	-1.96975800	3.51962200	8.00598400
H	0	-1.07612400	5.03227700	7.81797800
H	0	-0.20493500	3.53651300	8.23337300
H	0	0.53664500	4.07097200	4.55659700
H	0	1.32531800	3.98636600	6.10069000
H	0	0.37312700	5.40822900	5.86103900
O	0	2.67551400	2.55850400	3.59922300
O	0	4.82995700	4.96422800	3.68444000
O	0	5.43204000	2.13989600	3.52383400
Al	0	4.21790500	3.18347200	4.21250300
Cl	0	4.13431700	3.48474300	6.32308700

H	0	4.58518900	5.60364500	4.37372300
Al	0	-1.34962600	1.22556000	4.76170400
O	0	-3.02194400	0.66521900	5.42578500
C	0	-3.42417500	-0.02153400	6.64962700
C	0	-3.54056800	-1.50412800	6.36261400
H	0	-4.41034500	0.38957000	6.90525000
C	0	-2.44731700	0.30039600	7.76308400
H	0	-4.22298000	-1.68347500	5.52900500
H	0	-3.91601000	-2.01843500	7.25208500
H	0	-2.55956900	-1.92054500	6.11671800
H	0	-2.79065900	-0.16477300	8.69077900
H	0	-2.36100800	1.37824100	7.91121600
H	0	-1.45991200	-0.11060000	7.52573800
Al	0	-0.04348900	-1.45420400	4.02634900
O	0	-0.19468400	0.28086900	3.95009700
Cl	0	0.19806900	-1.91805200	6.15454000
C	0	2.13776700	0.58117200	5.87703700
C	0	1.77099400	0.79022900	7.26178100
H	0	1.56771900	1.11292200	5.10885000
C	0	3.25152500	-0.22326900	5.44101100
H	0	2.14803500	0.02300100	7.93743200
H	0	0.71073100	1.02605000	7.37304500
H	0	2.31567100	1.73774700	7.46798300
H	0	2.75872800	-1.07260400	4.90866100
H	0	3.88311200	-0.61208700	6.23818700
H	0	3.82021400	0.27168100	4.64217200

$Im2^{B\text{-}OiPr}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97259900
Si	-1	0.00000000	-1.92000000	-1.97259900
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000

Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010100	3.84010000	-0.61490000
Si	-1	-3.84010100	0.00000100	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	-0.00000200	3.84010000	-0.61490200
Si	-1	-0.00000200	0.00000100	-0.61490100
Si	-1	-0.00000100	-3.84010000	-0.61489800
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010200	0.00000000	-0.61490000
Si	-1	3.84010200	-3.84010100	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76009700	3.84019800	0.74280000
Si	-1	-5.76009600	0.00000100	0.74289900
Si	-1	-5.76010000	-3.84020000	0.74269900
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000100	7.68020000	0.74280000
Si	-1	-1.91989600	3.84010000	0.74280300
Si	-1	-1.92009700	-0.00000300	0.74290000
Si	-1	-1.92000100	-3.84010000	0.74279800
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92010000	3.84010000	0.74280100
Si	-1	1.92000000	-0.00000200	0.74279500
Si	-1	1.92000200	-3.84010000	0.74279100
Si	-1	1.91999900	-7.68019900	0.74280400
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010100	0.74279900
Si	-1	5.76009400	-0.00000300	0.74279900
Si	-1	5.76009100	-3.84009300	0.74279500
Si	-1	5.76010200	-7.68019900	0.74280300

H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960100	3.84790100	0.03190100
H	-1	-7.05810100	0.00000000	0.02880200
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000

H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150100	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810200	0.00000100	0.02890400
H	-1	7.05960300	-3.84790200	0.03190500
H	-1	7.00579900	-7.40190000	-0.01410100
H	-1	5.87799900	-8.93300100	1.52979900
Si	0	-4.99774500	5.77308200	2.04774200
Si	0	-5.08487800	1.90654000	1.90234100
Si	0	-4.97309300	-1.93112700	1.99715500
Si	0	-5.03961000	-5.75564900	1.93861400
Si	0	-2.42239400	5.74532200	2.02998500
Si	0	-2.65749900	1.95724600	1.87638200
Si	0	-2.43843200	-1.94854000	2.02605100
Si	0	-2.60214600	-5.74727400	1.93625700
Si	0	2.38693100	5.76397700	1.94594600
Si	0	2.68880100	2.00556400	2.00210400
Si	0	2.42895200	-1.92380400	1.97447900
Si	0	2.60793300	-5.74091600	1.93928900
Si	0	4.83367700	5.65086800	1.98246900
Si	0	5.11481300	1.91403100	1.90794900
Si	0	4.94372500	-1.94504800	1.99352400
Si	0	5.04505300	-5.75319900	1.93810700
O	0	-5.61445200	5.85124800	3.59110700
O	0	-5.33989100	1.82795400	3.54658000
O	0	-5.39580600	-2.02178000	3.62534800
O	0	-5.25504500	-5.64972000	3.60975200
O	0	-1.45225600	5.69458000	3.39405500
O	0	-2.47914400	2.20913500	3.59157500
O	0	-1.56117600	-2.07888300	3.43441800
O	0	-2.38995700	-5.68313400	3.60601500
O	0	1.64943700	5.83888200	3.42476300
O	0	1.54899900	-1.92372400	3.37910000
O	0	2.40630900	-5.60966400	3.60699700
O	0	5.25440100	-2.09989300	3.64179900

O	0	5.26865900	-5.60481700	3.60371400
H	0	-5.35811300	5.18091700	4.23863200
H	0	-6.32271100	-2.19161400	3.82774000
Al	0	-4.00333800	1.99188500	4.61642600
Al	0	-3.81802900	-5.49087500	4.53543600
Cl	0	-4.36467100	3.48909600	6.07846200
Cl	0	-3.82903900	-5.22990400	6.59273400
Al	0	-0.02702200	-1.33308800	3.83753200
Al	0	0.06888600	6.11178200	4.08154100
Cl	0	0.43953700	-1.54292700	6.18093600
Cl	0	-0.01368100	7.78520000	5.36558600
Al	0	3.83759200	-5.31025900	4.50682800
Cl	0	3.85247100	-4.78392800	6.51275200
H	0	6.16498200	-2.25316700	3.91863300
Al	0	-1.39283200	1.27114100	4.74314500
O	0	-3.06155500	0.61093700	5.33608900
O	0	-0.82926100	2.23513400	6.04882500
O	0	-0.25679100	0.36413200	3.86138200
C	0	-3.48796900	-0.11659600	6.52311300
C	0	-3.37178300	-1.60360200	6.25742800
C	0	-0.81408500	3.62707000	6.22913000
C	0	-0.82573000	3.95186500	7.71404600
C	0	1.78780800	-0.18932200	6.25058300
C	0	1.58726800	0.54254600	7.55570300
H	0	-4.54632900	0.14269900	6.66360000
C	0	-2.69734600	0.34501300	7.73222800
H	0	-3.93752200	-1.87799900	5.36434900
H	0	-3.75940500	-2.16180600	7.11408700
H	0	-2.32558300	-1.88743300	6.11322200
H	0	-1.69766200	4.08868400	5.76203800
C	0	0.42872900	4.17861200	5.54525100
H	0	-1.73146800	3.54939600	8.17307800
H	0	-0.80828700	5.03353700	7.87935100
H	0	0.04656400	3.50479400	8.20187800
H	0	1.52031600	0.43163200	5.39153400
C	0	3.12506800	-0.86807400	6.08803000
H	0	1.73955500	-0.12202400	8.41018700
H	0	0.60183400	1.01017600	7.59982700

H	0	2.34264200	1.33620700	7.59596400
H	0	-3.07452900	-0.15989600	8.62549100
H	0	-2.78208400	1.42517700	7.86709600
H	0	-1.63854300	0.09148000	7.61633300
H	0	3.18164400	-1.43867200	5.16014000
H	0	3.34392300	-1.52122600	6.93660100
H	0	3.88527900	-0.07855800	6.05160500
H	0	0.41172000	3.97247400	4.46302400
H	0	1.34360000	3.68501800	5.88907100
H	0	0.58517300	5.23736500	5.83309400
O	0	2.67857000	2.56225200	3.59284300
O	0	4.83753600	4.95034800	3.68113200
O	0	5.44942400	2.14480100	3.51926100
Al	0	4.21820900	3.14719500	4.24044300
Cl	0	4.15255600	3.51859900	6.33132800
H	0	4.60962500	5.58070800	4.38414000

P1$^{B\text{-}OiPr}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010100	3.84009900	-0.61489700
Si	-1	-3.84010100	-0.00000200	-0.61490000
Si	-1	-3.84010000	-3.84010100	-0.61490100
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490200
Si	-1	0.00000200	3.84010100	-0.61489700

Si	-1	0.00000000	-0.00000200	-0.61489900
Si	-1	0.00000000	-3.84010100	-0.61490200
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020200	-0.61490000
Si	-1	3.84010000	3.84010300	-0.61489900
Si	-1	3.84010000	-0.00000200	-0.61489900
Si	-1	3.84010000	-3.84010100	-0.61490100
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76009900	7.68020100	0.74280200
Si	-1	-5.76009800	3.84019900	0.74279400
Si	-1	-5.76009600	0.00000000	0.74289900
Si	-1	-5.76010100	-3.84020000	0.74270100
Si	-1	-5.76010100	-7.68020000	0.74279900
Si	-1	-1.92000200	7.68019900	0.74280300
Si	-1	-1.91990100	3.84010200	0.74279000
Si	-1	-1.92010000	0.00000500	0.74290000
Si	-1	-1.91999900	-3.84009800	0.74280400
Si	-1	-1.92000100	-7.68020000	0.74279900
Si	-1	1.92000300	7.68019700	0.74280400
Si	-1	1.91999900	3.84009400	0.74279800
Si	-1	1.91999900	0.00000500	0.74280000
Si	-1	1.91999900	-3.84009800	0.74280300
Si	-1	1.92000000	-7.68020000	0.74279900
Si	-1	5.76010200	7.68020100	0.74280300
Si	-1	5.76009600	3.84009600	0.74279300
Si	-1	5.76010200	0.00000500	0.74279800
Si	-1	5.76009900	-3.84010100	0.74280100
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000

H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420100
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85869900	-1.53420100
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410100
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960200	3.84790100	0.03190400
H	-1	-7.05810100	0.00000000	0.02880200
H	-1	-7.05950000	-3.84760000	0.03179900
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90149800	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90149800	8.88670000	1.61879900
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87619900	8.93250000	1.53079900
H	-1	7.00649900	7.40340000	-0.01330100
H	-1	7.05950200	3.84760100	0.03180300
H	-1	7.05810100	-0.00000100	0.02890100
H	-1	7.05960000	-3.84790000	0.03189900
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000

Si	0	-5.00207800	5.77923700	2.04722300
Si	0	-5.08178400	1.90197800	1.90880800
Si	0	-4.97349700	-1.93634300	1.99511600
Si	0	-5.04645800	-5.75346200	1.93848900
Si	0	-2.42414500	5.74563000	2.03481100
Si	0	-2.64901500	1.95480200	1.90333700
Si	0	-2.47281000	-1.94663800	1.97940900
Si	0	-2.60895000	-5.74188100	1.94168200
Si	0	2.38937000	5.76227300	1.94876100
Si	0	2.70779300	2.02345300	2.00074000
Si	0	2.42943600	-1.92798300	1.98578800
Si	0	2.60925500	-5.74467200	1.93847600
Si	0	4.83964000	5.65679800	1.98024500
Si	0	5.12625400	1.91723300	1.91723200
Si	0	4.95385400	-1.93951600	2.00093100
Si	0	5.04497700	-5.75686700	1.93821300
O	0	-5.63562200	5.87707100	3.57930700
O	0	-5.34076400	1.77647000	3.54798000
O	0	-5.28950500	-2.06146300	3.64534200
O	0	-5.27080700	-5.60563100	3.60469100
O	0	-1.45583300	5.67873800	3.39801400
O	0	-2.46512700	2.13547600	3.62555600
O	0	-1.59151200	-2.03263100	3.39387700
O	0	-2.40778800	-5.61906400	3.61034900
O	0	1.64238900	5.82348100	3.42239200
O	0	1.48921300	-1.92023000	3.37065000
O	0	2.40416000	-5.64663500	3.60665100
O	0	5.28124400	-2.05098000	3.64012400
O	0	5.26441400	-5.64896800	3.60543200
H	0	-5.36387500	5.22883500	4.24408200
H	0	-6.20306900	-2.21780000	3.91048000
Al	0	-4.02692100	2.01085300	4.63346200
Al	0	-3.83954100	-5.32205900	4.50946700
Cl	0	-4.41527400	3.68304500	5.89243300
Cl	0	-3.85769100	-4.78082000	6.51280100
Al	0	-0.06724100	-1.27546000	3.71702600
Al	0	0.06471500	6.15169800	4.05971900
Cl	0	-0.02693000	7.96306600	5.14122600

Al	0	3.83536800	-5.43911700	4.53395500
Cl	0	3.83880300	-5.11499400	6.57891600
H	0	6.19925100	-2.07920900	3.93101100
Al	0	-1.42168500	1.34160400	4.93603100
O	0	-3.10790900	0.69122700	5.47286700
O	0	-0.99355400	2.46304800	6.15283500
O	0	-0.23655600	0.26341500	4.37304400
C	0	-3.38911400	-0.11447700	6.64718000
C	0	-2.34083600	-1.21004700	6.71451500
C	0	-0.98009200	3.86100300	6.24494700
C	0	-1.18234000	4.27640600	7.69268400
H	0	-4.37157600	-0.56559300	6.47207200
C	0	-3.40735900	0.76508500	7.88551900
H	0	-2.32846600	-1.78023900	5.78109000
H	0	-2.56167600	-1.89385500	7.53724000
H	0	-1.34902600	-0.77513100	6.89650700
H	0	-1.78752600	4.29727500	5.63865400
C	0	0.34844900	4.36428600	5.69155700
H	0	-2.14954500	3.90890700	8.04379500
H	0	-1.16849300	5.36599700	7.79598600
H	0	-0.39295200	3.84739900	8.31717000
H	0	-3.59432300	0.15277700	8.77163100
H	0	-4.18862900	1.52677700	7.82035300
H	0	-2.44302300	1.27102500	7.99482100
H	0	0.48172400	4.07039600	4.63795600
H	0	1.21032400	3.91445100	6.19551900
H	0	0.47302200	5.44580800	5.90811700
O	0	2.69544800	2.62047000	3.56888700
O	0	4.87817100	4.97160900	3.66702400
O	0	5.45237900	2.15843700	3.52585500
Al	0	4.22845200	3.17112400	4.25406300
Cl	0	4.15294200	3.65566800	6.31436100
H	0	4.68180400	5.59595000	4.38467000

TS2$^{B\text{-}OiPr}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000

Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84020000	0.74280000
Si	-1	-5.76010000	0.00000000	0.74290000
Si	-1	-5.76010000	-3.84020000	0.74270000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.91990000	3.84010000	0.74280000
Si	-1	-1.92010000	0.00000000	0.74290000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68020000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000

Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000

H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02880000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.01121700	5.78115600	2.04294600
Si	0	-5.06923000	1.90293700	1.90690500
Si	0	-4.95573300	-1.93688900	1.99183500
Si	0	-5.03587800	-5.75024100	1.94171000
Si	0	-2.42886800	5.74636500	2.03191000
Si	0	-2.62895900	1.93719000	1.89984200
Si	0	-2.44937100	-1.94719400	2.00554600
Si	0	-2.59960800	-5.74429200	1.93776400
Si	0	2.39064200	5.76112200	1.94081000
Si	0	2.69818600	2.00927900	1.98763700
Si	0	2.36643900	-1.92392500	1.98948200
Si	0	2.60369600	-5.74333300	1.94081100
Si	0	4.83707300	5.66015400	1.96983900
Si	0	5.12047400	1.91323000	1.90896500
Si	0	4.91367400	-1.94320700	2.00017200
Si	0	5.03846600	-5.75065300	1.94180900
O	0	-5.65301800	5.89805500	3.56965100
O	0	-5.31912800	1.81276300	3.55187300
O	0	-5.29403200	-2.04804600	3.63965900
O	0	-5.24378100	-5.59316500	3.60795700
O	0	-1.44966300	5.69238600	3.39607700

O	0	-2.41282000	2.04399000	3.63371500
O	0	-1.66528400	-2.07243800	3.43689700
O	0	-2.38788300	-5.64636300	3.60169900
O	0	1.65823000	5.81423300	3.42594800
O	0	1.45928800	-1.89402900	3.35335100
O	0	2.40024000	-5.61862400	3.60439900
O	0	5.24661600	-2.05687400	3.64959500
O	0	5.25173000	-5.58007300	3.60506300
H	0	-5.39851400	5.24268800	4.23404800
H	0	-6.19710700	-2.27503800	3.88859300
Al	0	-3.99437400	2.06561800	4.61559800
Al	0	-3.80536800	-5.34048200	4.51872600
Cl	0	-4.36465600	3.79100400	5.81559000
Cl	0	-3.85139800	-4.89115700	6.54160500
Al	0	-0.10498400	-1.70692500	4.19364100
Al	0	0.07172200	6.20820000	4.01100600
Cl	0	0.20568200	-2.86927900	5.99295200
Cl	0	0.02440200	8.07411400	4.99414400
Al	0	3.81833500	-5.29058400	4.51467100
Cl	0	3.88717200	-4.73927500	6.51056700
H	0	6.14516300	-2.29190000	3.90858000
Al	0	-1.42064200	1.18631400	4.95549500
O	0	-3.14641700	0.79825500	5.57851800
O	0	-0.69035900	2.35424900	6.00837000
O	0	-0.26218000	-0.02372500	4.67358600
C	0	-3.59077900	0.00950000	6.71551700
C	0	-2.77312900	-1.26263300	6.74345300
C	0	-0.92837900	3.72959600	6.17126900
C	0	-1.28915100	4.04089300	7.61503900
C	0	2.17674200	0.75234400	6.00661900
C	0	1.38940600	0.40678900	7.11198200
H	0	-4.64246200	-0.22688300	6.51861000
C	0	-3.45371500	0.83467500	7.98188800
H	0	-2.82798500	-1.78221100	5.78251700
H	0	-3.13416400	-1.93538500	7.52482400
H	0	-1.72196700	-1.03900300	6.95717500
H	0	-1.74225900	4.07026200	5.51729200
C	0	0.33589800	4.46268000	5.74105400

H	0	-2.20224100	3.51170100	7.89433800
H	0	-1.45995400	5.11250700	7.75730100
H	0	-0.47884900	3.72190300	8.27977900
H	0	1.89841700	1.64984000	5.44980600
C	0	3.17266200	-0.12887600	5.40311500
H	0	1.68335400	-0.44582100	7.71751500
H	0	0.66920000	0.02608800	6.25417400
H	0	0.79183000	1.19611400	7.56260600
H	0	-3.78095700	0.24963700	8.84528600
H	0	-4.05189500	1.74866100	7.93242600
H	0	-2.40388000	1.11215600	8.12694600
H	0	2.62650300	-0.64023000	4.58391500
H	0	3.55586600	-0.89457600	6.07742500
H	0	3.97833800	0.43061300	4.91645000
H	0	0.61206700	4.17464000	4.71613100
H	0	1.20703500	4.19141300	6.34778900
H	0	0.22644600	5.55203300	5.92870900
O	0	2.68046500	2.58619800	3.58184800
O	0	4.83681700	4.97897500	3.68984300
O	0	5.43664500	2.15858600	3.52813300
Al	0	4.21936500	3.20111600	4.21526100
Cl	0	4.06907400	3.47875800	6.32261800
H	0	4.58732400	5.62102500	4.37495500

$Im3^{B\text{-}OiPr}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97259900
Si	-1	0.00000000	-1.92000000	-1.97259900
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.91999900	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000

Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010100	3.84009900	-0.61489900
Si	-1	-3.84010100	-0.00000100	-0.61490100
Si	-1	-3.84010000	-3.84010100	-0.61490100
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000500	3.84010000	-0.61490100
Si	-1	-0.00000300	-0.00000200	-0.61490100
Si	-1	-0.00000400	-3.84010000	-0.61490300
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020100	-0.61490100
Si	-1	3.84010100	3.84010300	-0.61490200
Si	-1	3.84010100	0.00000000	-0.61489700
Si	-1	3.84010100	-3.84010100	-0.61489800
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76009900	7.68020000	0.74280000
Si	-1	-5.76009800	3.84019800	0.74279700
Si	-1	-5.76009500	-0.00000100	0.74289900
Si	-1	-5.76010000	-3.84020000	0.74270000
Si	-1	-5.76010000	-7.68020100	0.74279900
Si	-1	-1.91999900	7.68020000	0.74280100
Si	-1	-1.91990400	3.84010300	0.74279200
Si	-1	-1.92009800	0.00000600	0.74290400
Si	-1	-1.91999500	-3.84009900	0.74280900
Si	-1	-1.92000300	-7.68020000	0.74279800
Si	-1	1.92000000	7.68020200	0.74279800
Si	-1	1.91999800	3.84009500	0.74281000
Si	-1	1.92000000	0.00000100	0.74279000
Si	-1	1.92000000	-3.84009700	0.74279700
Si	-1	1.92000000	-7.68020000	0.74280200
Si	-1	5.76010000	7.68019900	0.74280000
Si	-1	5.76009500	3.84009700	0.74280600
Si	-1	5.76010100	-0.00000100	0.74279500
Si	-1	5.76009800	-3.84009900	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000

H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960200	3.84790100	0.03190300
H	-1	-7.05810100	0.00000100	0.02880200
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90149900	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150100	-8.88670000	1.61890000

H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340100	-0.01330000
H	-1	7.05949900	3.84760100	0.03179800
H	-1	7.05810100	0.00000000	0.02890300
H	-1	7.05960100	-3.84790000	0.03190100
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00484000	5.78035400	2.04556500
Si	0	-5.08110300	1.90227000	1.90202500
Si	0	-4.97050000	-1.93507900	1.98925800
Si	0	-5.03803100	-5.75247500	1.94245000
Si	0	-2.42402100	5.74530300	2.03511100
Si	0	-2.64053600	1.92814000	1.89207300
Si	0	-2.47647700	-1.93260100	1.98801500
Si	0	-2.60284500	-5.74422200	1.93831800
Si	0	2.39226000	5.76330800	1.94509900
Si	0	2.71439300	2.02541100	1.99845900
Si	0	2.37632800	-1.92516900	1.99973900
Si	0	2.60625800	-5.74321500	1.93897000
Si	0	4.84229500	5.66174300	1.97186800
Si	0	5.13203100	1.91516000	1.91438800
Si	0	4.92712400	-1.94663800	2.00621000
Si	0	5.04075200	-5.75257100	1.94007100
O	0	-5.64060300	5.88389400	3.57688400
O	0	-5.34827100	1.79100600	3.54487400
O	0	-5.30178700	-2.04312100	3.63912200
O	0	-5.24741600	-5.60429700	3.60923200
O	0	-1.44991200	5.67435600	3.39927700
O	0	-2.42994600	1.95157000	3.64123000
O	0	-1.70511400	-1.95823500	3.44074300
O	0	-2.39024200	-5.63513400	3.60279600
O	0	1.64578900	5.83441900	3.42219300
O	0	1.43972000	-1.92624800	3.35311500
O	0	2.40162100	-5.62189400	3.60264300
O	0	5.28630400	-2.09467700	3.64159300
O	0	5.25391100	-5.60410900	3.60410500
H	0	-5.36466000	5.23710000	4.24057100
H	0	-6.20136800	-2.28204900	3.88984700

Al	0	-4.02898300	2.00109600	4.61563500
Al	0	-3.81116900	-5.36631900	4.52617400
Cl	0	-4.31478700	3.72422800	5.83010000
Cl	0	-3.86693500	-4.94151000	6.55401900
Al	0	-0.10751200	-1.89334800	4.16852800
Al	0	0.06855500	6.15348000	4.05604500
Cl	0	0.01451500	-3.14646500	5.88498000
Cl	0	-0.02844500	7.90242400	5.23037800
Al	0	3.82351900	-5.33159900	4.52227200
Cl	0	3.88034100	-4.85525600	6.53572100
H	0	6.19435200	-2.30516200	3.88723200
Al	0	-1.50111000	1.11342800	4.98226600
O	0	-3.19836900	0.68801600	5.56035700
O	0	-0.70651500	2.21529100	6.02032600
O	0	-0.26170100	-0.12606800	4.72406100
C	0	-3.62311900	-0.08740400	6.72213600
C	0	-2.77020200	-1.33563700	6.76442300
C	0	-0.85028200	3.61053000	6.16857300
C	0	-1.12695100	3.95276500	7.62265500
C	0	2.36569900	0.58723300	6.06657300
C	0	1.64881500	0.01543200	7.04093800
H	0	-4.66739800	-0.35202200	6.52648800
C	0	-3.49773100	0.76842800	7.96839300
H	0	-2.81172900	-1.86546300	5.80860200
H	0	-3.11311500	-2.01196000	7.55066300
H	0	-1.72543000	-1.08205300	6.98335000
H	0	-1.67856900	3.98381500	5.55067500
C	0	0.42805400	4.26409700	5.66409200
H	0	-2.06558700	3.49383100	7.94195200
H	0	-1.21316600	5.03514400	7.76032300
H	0	-0.31549400	3.57707600	8.25383700
H	0	2.16082700	1.62757500	5.81204400
C	0	3.44284800	-0.10419600	5.28718700
H	0	1.80414300	-1.02268200	7.32512400
H	0	0.53167100	0.11649500	5.26999300
H	0	0.89144700	0.58129300	7.57788600
H	0	-3.79646400	0.18886600	8.84550900
H	0	-4.12497900	1.66185200	7.91138700

H	0	-2.45577000	1.08109500	8.09609100
H	0	3.25726600	-0.02446400	4.20832500
H	0	3.50781200	-1.16552500	5.53732300
H	0	4.42032600	0.35774600	5.47058500
H	0	0.62742900	4.00302500	4.61485200
H	0	1.31582300	3.92513100	6.20963500
H	0	0.40271700	5.35081300	5.88911100
O	0	2.70136100	2.63091500	3.57586300
O	0	4.88375500	4.98466100	3.66401400
O	0	5.46383200	2.16878800	3.52197200
Al	0	4.24678000	3.19281300	4.23816200
Cl	0	4.19809200	3.65193200	6.30924900
H	0	4.70108100	5.61096500	4.38342700

P2$^{B\text{-}OiPr}$

Atom	Fix/Relax	X	Y	Z
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97259900
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260100
Si	-1	0.00000100	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010100	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.91999900	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010100	3.84010000	-0.61489900
Si	-1	-3.84010200	-0.00000100	-0.61489900
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000100	7.68020000	-0.61490000
Si	-1	-0.00000200	3.84010300	-0.61489600
Si	-1	0.00000100	-0.00000300	-0.61490000
Si	-1	0.00000100	-3.84010000	-0.61489900
Si	-1	0.00000000	-7.68020000	-0.61490000

Si	-1	3.84009900	7.68020100	-0.61489900
Si	-1	3.84009900	3.84010100	-0.61490000
Si	-1	3.84010100	-0.00000400	-0.61489900
Si	-1	3.84009900	-3.84010000	-0.61490100
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010300	3.84019600	0.74280000
Si	-1	-5.76009200	-0.00000100	0.74289900
Si	-1	-5.76010100	-3.84020000	0.74270000
Si	-1	-5.76010100	-7.68020100	0.74280000
Si	-1	-1.92000200	7.68019900	0.74280100
Si	-1	-1.91990000	3.84010300	0.74279600
Si	-1	-1.92009800	0.00000600	0.74289400
Si	-1	-1.92000300	-3.84009800	0.74279900
Si	-1	-1.92000100	-7.68020000	0.74280000
Si	-1	1.91999800	7.68020000	0.74280300
Si	-1	1.92000800	3.84009500	0.74279700
Si	-1	1.91999600	0.00000900	0.74280400
Si	-1	1.91999800	-3.84010600	0.74280100
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010900	7.68019300	0.74280100
Si	-1	5.76008200	3.84010200	0.74279100
Si	-1	5.76010800	0.00000800	0.74280000
Si	-1	5.76010000	-3.84010300	0.74279900
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000

H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410100
H	-1	-5.87799900	8.93300000	1.52980000
H	-1	-7.05960100	3.84790100	0.03190200
H	-1	-7.05810100	0.00000000	0.02880200
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90149900	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150200	8.88670000	1.61879900
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87619500	8.93250100	1.53079900
H	-1	7.00650000	7.40340100	-0.01330000
H	-1	7.05950300	3.84759800	0.03180500
H	-1	7.05810200	-0.00000300	0.02890300
H	-1	7.05959900	-3.84789900	0.03189900
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00527300	5.78047300	2.04563600
Si	0	-5.08349000	1.90178000	1.89881600
Si	0	-4.96550600	-1.93449700	1.99299200

Si	0	-5.03887700	-5.75310700	1.94220100
Si	0	-2.42540500	5.74559700	2.03540000
Si	0	-2.64494600	1.93130000	1.88585400
Si	0	-2.46489200	-1.92802400	1.99666300
Si	0	-2.60349600	-5.74443000	1.93871100
Si	0	2.38883500	5.76255600	1.94433200
Si	0	2.70549800	2.00877200	1.98719800
Si	0	2.39868400	-1.92154400	1.99159200
Si	0	2.60501900	-5.74610100	1.93829200
Si	0	4.83539100	5.65265200	1.98081900
Si	0	5.12571400	1.91568100	1.91366300
Si	0	4.93579000	-1.94012400	2.00116900
Si	0	5.03891000	-5.75515100	1.94127800
O	0	-5.64176600	5.88409600	3.57682900
O	0	-5.35175900	1.78651500	3.54182100
O	0	-5.29933200	-2.04296300	3.64253000
O	0	-5.24973500	-5.60745800	3.60932600
O	0	-1.45255800	5.67674900	3.40015200
O	0	-2.43826700	1.97687800	3.63562300
O	0	-1.67845400	-1.93156700	3.44767200
O	0	-2.39155600	-5.63154900	3.60349300
O	0	1.64441500	5.82636300	3.42231600
O	0	1.47569500	-1.89927200	3.35622800
O	0	2.39399400	-5.65935900	3.60269300
O	0	5.27980900	-2.04478500	3.63792500
O	0	5.24705400	-5.64266600	3.60769900
H	0	-5.36677600	5.23809900	4.24149100
H	0	-6.20024900	-2.27880100	3.89163300
Al	0	-4.03432100	2.00678600	4.61105200
Al	0	-3.81415900	-5.36884200	4.52627300
Cl	0	-4.33301200	3.71649300	5.83903300
Cl	0	-3.85992900	-4.93698200	6.55254600
Al	0	-0.07346200	-1.85268500	4.15682500
Al	0	0.06685700	6.16204300	4.05204100
Cl	0	0.05177900	-3.02694800	5.92086000
Cl	0	-0.02064100	7.94435300	5.17584000
Al	0	3.81618700	-5.46079500	4.54621600
Cl	0	3.86272400	-5.21834500	6.59931400

H	0	6.19752000	-2.15521800	3.90917600
Al	0	-1.49901200	1.14663300	4.96806200
O	0	-3.18333700	0.69457100	5.54886900
O	0	-0.69038500	2.24159300	5.99630600
O	0	-0.20033600	-0.02955800	4.60782600
C	0	-3.61554100	-0.08094000	6.71040200
C	0	-2.76256300	-1.32705200	6.75040000
C	0	-0.86541500	3.63192600	6.16976700
C	0	-1.15638400	3.94527700	7.62722900
H	0	-4.65931000	-0.34233200	6.50783100
C	0	-3.49359900	0.77124900	7.95898300
H	0	-2.81623300	-1.86427200	5.79968200
H	0	-3.09000400	-1.99878300	7.54706900
H	0	-1.71670300	-1.06645500	6.95494900
H	0	-1.69736900	3.99749100	5.55234900
C	0	0.40228600	4.31619000	5.68187400
H	0	-2.08823100	3.46462800	7.93373400
H	0	-1.26500900	5.02367300	7.77936800
H	0	-0.34229700	3.57574200	8.25772700
H	0	0.65002800	0.36494600	4.86733000
H	0	-3.80330800	0.18989600	8.83110200
H	0	-4.11540600	1.66826800	7.90095800
H	0	-2.45069600	1.07523100	8.09779600
H	0	0.60893300	4.06073100	4.63240700
H	0	1.29361400	3.98371600	6.22376700
H	0	0.35342900	5.40039600	5.91453000
O	0	2.66225100	2.55360200	3.58353600
O	0	4.83563800	4.95186500	3.66938100
O	0	5.43720000	2.15395400	3.52564400
Al	0	4.19931000	3.14871500	4.24721900
Cl	0	4.11516700	3.61485800	6.31354700
H	0	4.62360200	5.57681700	4.38218100

Im1$^{B\text{-}OEt}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97259900
Si	-1	-3.84010000	-1.92000000	-1.97259900

Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97259900
Si	-1	0.00000000	-1.92000000	-1.97259900
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.91999900	-1.97260100
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010200	3.84009900	-0.61490100
Si	-1	-3.84010200	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010200	-0.61490100
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000400	-0.00000100	-0.61490200
Si	-1	-0.00000100	-3.84009800	-0.61490300
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010200	0.00000300	-0.61489800
Si	-1	3.84010100	-3.84010000	-0.61489800
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010100	7.68020000	0.74279900
Si	-1	-5.76009400	3.84009700	0.74280000
Si	-1	-5.76019500	0.00000200	0.74279100
Si	-1	-5.76020000	-3.84010100	0.74280300
Si	-1	-5.76010100	-7.68020000	0.74279900
Si	-1	-1.92000000	7.68020000	0.74280100
Si	-1	-1.92000200	3.84009900	0.74279900
Si	-1	-1.91999800	0.00000300	0.74279200
Si	-1	-1.92000100	-3.84009700	0.74280700
Si	-1	-1.91999900	-7.68030100	0.74280000
Si	-1	1.92000100	7.68019900	0.74280000
Si	-1	1.92000100	3.84010000	0.74280000
Si	-1	1.91999300	-0.00000200	0.74280400
Si	-1	1.91999800	-3.84010700	0.74279900

Si	-1	1.92000000	-7.68019800	0.74280100
Si	-1	5.76010100	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74279800
Si	-1	5.76009900	0.00000200	0.74280200
Si	-1	5.76009900	-3.84009600	0.74279600
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000

H	-1	-7.05960200	3.84790100	0.03190300
H	-1	-7.05810300	-0.00000100	0.02890600
H	-1	-7.05949900	-3.84760000	0.03179900
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150100	-8.88670000	1.61880000
H	-1	1.90149900	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	-0.00000100	0.02890000
H	-1	7.05960100	-3.84790100	0.03190200
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00985500	5.77897200	2.04057500
Si	0	-5.04518400	1.89669400	1.93827500
Si	0	-4.96990800	-1.93678500	1.99061000
Si	0	-5.04116400	-5.75315100	1.94076400
Si	0	-2.44505600	5.74720400	2.02305800
Si	0	-2.61853300	1.92492400	1.83076700
Si	0	-2.46104100	-1.90488800	2.00538000
Si	0	-2.60653600	-5.74396800	1.93964800
Si	0	2.36001000	5.75451400	1.96205900
Si	0	2.70520800	2.00999700	1.97925300
Si	0	2.37672000	-1.92731600	2.00084500
Si	0	2.60665800	-5.74422600	1.93917300
Si	0	4.82229800	5.65005300	1.99160200
Si	0	5.12488600	1.91536300	1.91256500
Si	0	4.92278900	-1.94457600	2.00418900
Si	0	5.04132300	-5.75391500	1.93976100
O	0	-5.62932400	5.86546000	3.58049700
O	0	-5.17831800	1.76721000	3.60682000
O	0	-5.33361900	-2.06898400	3.63086300
O	0	-5.25561300	-5.60917500	3.60687500
O	0	-1.50115000	5.70432100	3.40181300
O	0	-2.30124100	1.93512500	3.53679100

O	0	-1.66431800	-1.77967100	3.44625600
O	0	-2.39905900	-5.62664600	3.60487900
O	0	1.57959000	5.78075700	3.42862600
O	0	1.44715200	-1.93960600	3.36281000
O	0	2.40120900	-5.63568100	3.60362100
O	0	5.25730300	-2.07423600	3.64434900
O	0	5.25506900	-5.62098700	3.60485300
H	0	-5.28260100	5.25921100	4.24963400
H	0	-6.22478000	-2.35947800	3.85618100
Al	0	-3.80598600	2.01107000	4.61943500
Al	0	-3.82291800	-5.37349000	4.52958900
Cl	0	-3.93388800	3.82388000	5.72834800
Cl	0	-3.88105400	-4.96230300	6.55854600
Al	0	-0.08182500	-1.76833500	4.20045700
Al	0	0.01924000	6.00929300	4.13408200
Cl	0	-0.14397600	-2.96778300	5.96016900
Cl	0	0.01112600	7.40335000	5.70401500
Al	0	3.82504600	-5.38080800	4.53085000
Cl	0	3.86618000	-4.98746900	6.56175700
H	0	6.17080800	-2.21775000	3.91538500
Al	0	-1.18021400	1.34055400	4.83969100
O	0	-2.77594600	0.88464300	5.63744200
O	0	-0.31492300	2.63644700	5.50184100
O	0	0.00008200	0.00142400	4.81129300
C	0	-2.99456400	0.08571000	6.82458600
C	0	-3.66532800	-1.21361600	6.44182800
C	0	-0.24527500	3.96967600	5.85398500
C	0	0.11610600	4.13756600	7.32074800
C	0	1.27780500	0.27407000	5.52415900
C	0	1.06533100	0.27872100	7.02134000
H	0	-3.59054500	0.68445600	7.51958100
H	0	-2.01304900	-0.09265900	7.27563800
H	0	-4.62489900	-1.03055400	5.94945700
H	0	-3.83485500	-1.82284500	7.33312800
H	0	-3.03088300	-1.77787000	5.75238800
H	0	-1.18832500	4.49591700	5.63532500
H	0	0.60733800	4.40744600	5.26301400
H	0	-0.67452000	3.69361200	7.93177400

H	0	0.21303400	5.19354900	7.58080500
H	0	1.05990000	3.62714300	7.52628900
H	0	1.64937900	1.22897500	5.15241500
H	0	1.96223400	-0.52059900	5.21798100
H	0	0.69333100	-0.68710200	7.36956900
H	0	0.37760700	1.07744400	7.31440400
H	0	2.02444000	0.47678500	7.50888000
O	0	2.66835200	2.57197700	3.56519700
O	0	4.83726700	4.95377800	3.68615100
O	0	5.43382000	2.15610300	3.52667000
Al	0	4.19532400	3.15325400	4.24694200
Cl	0	4.03100400	3.56538800	6.31824600
H	0	4.62007300	5.58048300	4.39586700

TS1$^{B\text{-}OEt}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000

Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76020000	0.00000000	0.74280000
Si	-1	-5.76020000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68030000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000

H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00690300	5.77629500	2.04105500
Si	0	-5.05253100	1.90244500	1.93202900
Si	0	-4.96234900	-1.93986000	1.99269900

Si	0	-5.03915300	-5.75132500	1.93964000
Si	0	-2.44124000	5.74561400	2.02075100
Si	0	-2.63436700	1.95215600	1.83132600
Si	0	-2.44629700	-1.94215300	2.01048700
Si	0	-2.60250900	-5.74401700	1.93865100
Si	0	2.35764000	5.75344200	1.96144900
Si	0	2.69506500	1.99824600	1.98311000
Si	0	2.39766400	-1.92926400	2.00181100
Si	0	2.60470900	-5.74345300	1.93937800
Si	0	4.82038300	5.65635400	1.97716000
Si	0	5.12111700	1.91486600	1.90592300
Si	0	4.92692800	-1.94326600	1.99727000
Si	0	5.04094400	-5.75246200	1.93913000
O	0	-5.61575400	5.86677600	3.58529800
O	0	-5.19175900	1.82566500	3.59871100
O	0	-5.33361800	-2.07112000	3.63069900
O	0	-5.25391200	-5.60166300	3.60618300
O	0	-1.49247900	5.71960000	3.40092500
O	0	-2.35567200	2.23114700	3.51913000
O	0	-1.61907100	-2.05127600	3.42895200
O	0	-2.39481300	-5.64710500	3.60488800
O	0	1.59089300	5.76431700	3.43736300
O	0	1.54058800	-1.95470600	3.40968800
O	0	2.40202200	-5.62830900	3.60585000
O	0	5.25192700	-2.05896200	3.64611300
O	0	5.26021100	-5.59956800	3.60405100
H	0	-5.30121000	5.23877800	4.25025400
H	0	-6.22992800	-2.34675300	3.85388800
Al	0	-3.82583800	2.09751800	4.61990500
Al	0	-3.81760800	-5.35739400	4.51993300
Cl	0	-4.10745700	3.76534400	5.91232100
Cl	0	-3.84805000	-4.92414200	6.54612300
Al	0	0.02736700	6.01059500	4.13338700
Cl	0	0.03502600	7.37992100	5.72435500
Al	0	3.82714400	-5.32753600	4.51448000
Cl	0	3.86414700	-4.82307900	6.52385500
H	0	6.15984400	-2.24286600	3.91276000
Al	0	-1.15606000	1.40594600	4.62942000

O	0	-2.74504900	0.91284800	5.48766700
O	0	-0.25109600	2.51810400	5.60276300
C	0	-2.95321800	0.17996700	6.71684500
C	0	-3.60027600	-1.15039100	6.40551500
C	0	-0.40410000	3.87065200	5.88111900
C	0	-0.26919600	4.15275600	7.36656400
H	0	-3.56924000	0.80407300	7.37297900
H	0	-1.97469500	0.04441500	7.18532700
H	0	-4.56989000	-1.01123700	5.91866300
H	0	-3.74409200	-1.72252200	7.32572600
H	0	-2.96101200	-1.72838500	5.73245000
H	0	-1.36108800	4.26719600	5.51006200
H	0	0.44664800	4.40316700	5.36143100
H	0	-1.05964800	3.61326800	7.89532100
H	0	-0.36813100	5.21929700	7.57695900
H	0	0.70352900	3.80937000	7.72867100
O	0	2.68688400	2.53807700	3.59164100
O	0	4.83194800	4.96527000	3.68575500
O	0	5.44783200	2.16034300	3.52136600
Al	0	4.21874400	3.17985100	4.21640200
Cl	0	4.08596400	3.55122700	6.31188100
H	0	4.59706800	5.59769100	4.38484300
Al	0	-0.05996400	-1.43975900	3.98981500
O	0	-0.11326800	0.30132900	3.87256900
Cl	0	0.05362200	-1.76585600	6.15976000
C	0	1.98189100	0.40460700	5.58532200
C	0	1.97043100	0.68441200	6.98829700
H	0	1.68687400	1.18281300	4.88325600
H	0	2.42845500	-0.50456200	5.17835500
H	0	2.13375200	-0.16463000	7.64540100
H	0	1.13450000	1.33646700	7.25968000
H	0	2.85198600	1.37634900	7.01369300

Im2$^{B\text{-}OEt}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010100	1.92000100	-1.97260100
Si	-1	-3.84010000	-1.92000200	-1.97260000

Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010100	-1.97260000
Si	-1	0.00000100	1.92000200	-1.97259800
Si	-1	0.00000100	-1.92000200	-1.97259900
Si	-1	0.00000000	-5.76010100	-1.97260000
Si	-1	3.84010000	5.76010100	-1.97259900
Si	-1	3.84010000	1.92000100	-1.97260000
Si	-1	3.84010000	-1.92000300	-1.97260000
Si	-1	3.84010100	-5.76009900	-1.97260000
Si	-1	-3.84010000	7.68019900	-0.61490000
Si	-1	-3.84009800	3.84009600	-0.61489700
Si	-1	-3.84009800	0.00000800	-0.61490200
Si	-1	-3.84009900	-3.84009300	-0.61489900
Si	-1	-3.84010000	-7.68020200	-0.61489900
Si	-1	0.00000000	7.68020000	-0.61489900
Si	-1	0.00000600	3.84009200	-0.61490000
Si	-1	-0.00000200	0.00000200	-0.61491900
Si	-1	-0.00001000	-3.84010400	-0.61490100
Si	-1	0.00000200	-7.68020100	-0.61489700
Si	-1	3.84010000	7.68019900	-0.61490000
Si	-1	3.84010100	3.84009700	-0.61490200
Si	-1	3.84009400	0.00000500	-0.61491700
Si	-1	3.84010200	-3.84009600	-0.61488500
Si	-1	3.84009900	-7.68020100	-0.61489900
Si	-1	-5.76009800	7.68020000	0.74280000
Si	-1	-5.76010400	3.84009400	0.74279600
Si	-1	-5.76020300	-0.00001000	0.74278800
Si	-1	-5.76020300	-3.84010200	0.74279500
Si	-1	-5.76010000	-7.68019900	0.74280000
Si	-1	-1.91999600	7.68019900	0.74279800
Si	-1	-1.92001500	3.84012000	0.74279200
Si	-1	-1.91998500	-0.00000700	0.74281800
Si	-1	-1.91999200	-3.84010500	0.74281700
Si	-1	-1.92001000	-7.68029400	0.74279100
Si	-1	1.91999900	7.68020100	0.74279800
Si	-1	1.91998700	3.84011400	0.74280100
Si	-1	1.92003300	-0.00001100	0.74284000
Si	-1	1.91996800	-3.84008400	0.74276500

Si	-1	1.92001600	-7.68020300	0.74280500
Si	-1	5.76010000	7.68019900	0.74279700
Si	-1	5.76009700	3.84010100	0.74280000
Si	-1	5.76010300	-0.00001300	0.74281800
Si	-1	5.76011300	-3.84011700	0.74279800
Si	-1	5.76010700	-7.68020100	0.74280300
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000100	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85869900	-1.53420100
H	-1	-7.00580000	7.40190000	-0.01409900
H	-1	-5.87799900	8.93300000	1.52980000

H	-1	-7.05960100	3.84790300	0.03190200
H	-1	-7.05810100	0.00000300	0.02890200
H	-1	-7.05950100	-3.84760000	0.03180200
H	-1	-5.87619900	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150100	8.88670000	1.61890100
H	-1	-1.90149500	-8.88669900	1.61880100
H	-1	1.90150100	8.88670000	1.61880000
H	-1	1.90149200	-8.88669900	1.61890100
H	-1	5.87620000	8.93250000	1.53080100
H	-1	7.00650100	7.40340000	-0.01329900
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05809300	0.00000400	0.02888800
H	-1	7.05959800	-3.84789500	0.03189700
H	-1	7.00579800	-7.40189800	-0.01410300
H	-1	5.87799900	-8.93300000	1.52980000
Si	0	-5.00488100	5.77662300	2.04252900
Si	0	-5.05601500	1.90451400	1.93113700
Si	0	-4.96779000	-1.93930000	1.99714300
Si	0	-5.04295200	-5.75249700	1.93887700
Si	0	-2.44038500	5.74239800	2.02649800
Si	0	-2.63987000	1.95615600	1.82636000
Si	0	-2.45461000	-1.94260400	2.01050900
Si	0	-2.60523900	-5.74302000	1.93849800
Si	0	2.35726400	5.75365100	1.96463600
Si	0	2.68668100	2.00373900	1.99642900
Si	0	2.41944600	-1.92722300	1.98296900
Si	0	2.60792700	-5.73798000	1.93875700
Si	0	4.82012900	5.64803900	1.99308600
Si	0	5.11249500	1.91523400	1.91128100
Si	0	4.93675100	-1.94857500	1.99533400
Si	0	5.04587500	-5.75054100	1.94061600
O	0	-5.61778200	5.86375400	3.58540000
O	0	-5.19627000	1.82727500	3.59701200
O	0	-5.32098900	-2.07394500	3.64006500
O	0	-5.26220000	-5.60336300	3.60661900
O	0	-1.50293400	5.69723900	3.41069300
O	0	-2.36725900	2.26137900	3.50547400

O	0	-1.59975000	-2.04015500	3.43495100
O	0	-2.39837200	-5.63173700	3.60653400
O	0	1.57747100	5.77462600	3.43109100
O	0	2.67190700	2.56454200	3.57874500
O	0	1.52749000	-1.94551400	3.38297100
O	0	2.40593000	-5.57198200	3.60345600
O	0	4.83924200	4.94735400	3.68468400
O	0	5.43705200	2.14638800	3.52391500
O	0	5.23683800	-2.12457500	3.64408800
O	0	5.26592700	-5.57142300	3.60527100
H	0	-5.27443700	5.26155200	4.25991400
H	0	-6.22687900	-2.30560700	3.87501000
Al	0	-3.82812500	2.11552100	4.61249300
Al	0	-3.82653600	-5.33917300	4.51157300
Cl	0	-4.09801900	3.77656100	5.91052800
Cl	0	-3.83055100	-4.85130400	6.52815200
Al	0	-0.04879900	-1.32867900	3.81340200
Al	0	0.01830600	5.99782400	4.14258300
Cl	0	0.01068200	7.40607500	5.69985000
Al	0	3.83476300	-5.19804500	4.48012700
Al	0	4.19966900	3.14224000	4.25011500
Cl	0	3.81870300	-4.51950400	6.44359300
Cl	0	4.10404400	3.55689900	6.32814200
H	0	4.62648500	5.57224500	4.39721200
H	0	6.14750600	-2.27288700	3.92370400
Al	0	-1.15083600	1.50034300	4.63890400
O	0	-2.74630500	0.91353500	5.45649400
O	0	-0.41698300	2.59714300	5.72963900
O	0	-0.14086900	0.37644600	3.86992900
C	0	-2.90698000	0.24252600	6.72014300
C	0	-3.45799500	-1.14711900	6.48336100
C	0	-0.28162800	3.95224200	5.96428400
C	0	0.24712400	4.20398200	7.36582300
H	0	-3.56710500	0.85058100	7.34772000
H	0	-1.92520000	0.21402900	7.20496300
H	0	-4.43535800	-1.09914100	5.99479300
H	0	-3.56059600	-1.68556600	7.42886000
H	0	-2.79359300	-1.71310000	5.82352600

H	0	-1.23318400	4.48680200	5.81076400
H	0	0.50154800	4.34708500	5.24746300
H	0	-0.47184300	3.80524600	8.08567900
H	0	0.38264300	5.27059800	7.55316000
H	0	1.20354800	3.69209200	7.49365900
Cl	0	0.23716700	-1.72886700	6.14878600
C	0	1.77774200	-0.69323800	6.30586900
C	0	1.60494900	0.30877500	7.41870800
H	0	1.89057100	-0.22268800	5.32859700
H	0	2.55934000	-1.43344700	6.47055800
H	0	2.54041100	0.87249700	7.49961600
H	0	1.40795200	-0.17676300	8.37658000
H	0	0.81155600	1.02338500	7.18335100

P1$^{\textbf{B-OEt}}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000

Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76020000	0.00000000	0.74280000
Si	-1	-5.76020000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68030000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000

H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.02185400	5.78602100	2.03754500
Si	0	-5.05253700	1.90972000	1.94138700
Si	0	-4.97435300	-1.93858400	1.99105100

Si	0	-5.04511000	-5.75355600	1.93986400
Si	0	-2.45175600	5.74706700	2.02883300
Si	0	-2.62471000	1.94441100	1.86040900
Si	0	-2.47029400	-1.94396200	1.98209400
Si	0	-2.60840700	-5.74268400	1.94115300
Si	0	2.35089600	5.75299900	1.96949400
Si	0	2.71638300	2.02540800	2.00122900
Si	0	2.42140400	-1.92487800	1.98913400
Si	0	2.60923900	-5.74456400	1.93794800
Si	0	4.82559700	5.64788300	1.99505100
Si	0	5.13497200	1.91652400	1.92123500
Si	0	4.94965400	-1.94113300	2.00268900
Si	0	5.04487500	-5.75653300	1.93762300
O	0	-5.68635400	5.91395200	3.55336500
O	0	-5.20924000	1.86143500	3.60882100
O	0	-5.29789400	-2.05394100	3.63683700
O	0	-5.26549200	-5.60673200	3.60615900
O	0	-1.52086200	5.69993700	3.41338200
O	0	-2.35911800	2.11366700	3.56067000
O	0	-1.58917800	-2.00475700	3.39287500
O	0	-2.40468300	-5.62293800	3.60830200
O	0	1.55227600	5.75632200	3.42264900
O	0	1.48066800	-1.90206000	3.37163200
O	0	2.40427500	-5.64594200	3.60629500
O	0	5.28468500	-2.06529700	3.63978400
O	0	5.26543400	-5.64688300	3.60485100
H	0	-5.37070000	5.32245900	4.25006700
H	0	-6.21025700	-2.20915600	3.90554300
Al	0	-3.85823100	2.21726900	4.62430400
Al	0	-3.83377200	-5.33240000	4.51479800
Cl	0	-4.06937800	4.04473000	5.70261900
Cl	0	-3.83978700	-4.81901000	6.52330400
Al	0	-0.07030600	-1.26283400	3.75867100
Al	0	0.00165200	6.04745800	4.12932900
Cl	0	0.00320900	7.58319400	5.56331100
Al	0	3.83570500	-5.44523700	4.53438000
Cl	0	3.84248600	-5.12322400	6.57966700
H	0	6.20204400	-2.16788600	3.91560000

Al	0	-1.22043700	1.54606200	4.89539400
O	0	-2.86898000	1.15811800	5.72777500
O	0	-0.50102600	2.81786900	5.76563900
O	0	-0.22141700	0.23046500	4.51392700
C	0	-2.99547900	0.99964400	7.15506300
C	0	-1.90302900	0.08016200	7.65926000
C	0	-0.38034400	4.16502400	6.00812000
C	0	0.04324100	4.43411200	7.44262200
H	0	-3.98559900	0.57982900	7.35167600
H	0	-2.93130900	1.98964400	7.61921600
H	0	-1.95804100	-0.88901400	7.15682200
H	0	-2.01513300	-0.07791000	8.73447600
H	0	-0.91328600	0.51837000	7.48882000
H	0	-1.31105000	4.70753400	5.77886600
H	0	0.46715300	4.54816200	5.35898700
H	0	-0.74072600	4.07114100	8.11229300
H	0	0.18874500	5.50230700	7.61575100
H	0	0.96979500	3.89885600	7.65834900
O	0	2.69985700	2.60990900	3.56907300
O	0	4.87311700	4.95932500	3.67829700
O	0	5.45528200	2.15073600	3.53085000
Al	0	4.22631700	3.15736000	4.26555900
Cl	0	4.16931000	3.64082600	6.32470600
H	0	4.68212000	5.58187900	4.39905600

TS2$^{B\text{-}OEt}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000

Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76020000	0.00000000	0.74280000
Si	-1	-5.76020000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68030000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000

H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000

H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.01130000	5.77870000	2.03980000
Si	0	-5.04810000	1.90190000	1.93640000
Si	0	-4.96340000	-1.93980000	1.98960000
Si	0	-5.03770000	-5.75120000	1.94030000
Si	0	-2.44480000	5.74630000	2.02140000
Si	0	-2.62500000	1.94690000	1.84280000
Si	0	-2.44960000	-1.94010000	2.00420000
Si	0	-2.60170000	-5.74440000	1.93860000
Si	0	2.35690000	5.75290000	1.96450000
Si	0	2.70600000	2.00630000	1.96980000
Si	0	2.38110000	-1.92840000	2.01180000
Si	0	2.60450000	-5.74360000	1.93950000
Si	0	4.82150000	5.65420000	1.98550000
Si	0	5.12680000	1.91390000	1.90360000
Si	0	4.92010000	-1.94360000	2.00010000
Si	0	5.04030000	-5.75230000	1.93970000
O	0	-5.63020000	5.87710000	3.57860000
O	0	-5.18770000	1.82120000	3.60370000
O	0	-5.33620000	-2.06890000	3.62730000
O	0	-5.24990000	-5.60220000	3.60680000
O	0	-1.49810000	5.71470000	3.40200000
O	0	-2.33320000	2.16250000	3.54110000
O	0	-1.63690000	-2.03190000	3.42470000
O	0	-2.39200000	-5.65030000	3.60400000
O	0	1.58380000	5.77200000	3.43660000
O	0	2.69160000	2.57870000	3.56100000
O	0	1.51820000	-1.94440000	3.41280000
O	0	2.40100000	-5.62640000	3.60500000
O	0	4.83970000	4.96610000	3.69820000
O	0	5.44850000	2.15930000	3.51820000

O	0	5.25140000	-2.05860000	3.64680000
O	0	5.25720000	-5.59900000	3.60440000
H	0	-5.31180000	5.25730000	4.24950000
H	0	-6.22680000	-2.36410000	3.84830000
Al	0	-3.83000000	2.10770000	4.62990000
Al	0	-3.81310000	-5.37010000	4.52440000
Cl	0	-4.08520000	3.84510000	5.83580000
Cl	0	-3.85610000	-4.96540000	6.55550000
Al	0	-0.07730000	-1.58080000	4.12100000
Al	0	0.02080000	6.02380000	4.13050000
Cl	0	-0.02860000	-2.37210000	6.15510000
Cl	0	0.02040000	7.42580000	5.69290000
Al	0	3.82470000	-5.32670000	4.51680000
Al	0	4.22320000	3.17870000	4.22220000
Cl	0	3.86940000	-4.83200000	6.52830000
Cl	0	4.02990000	3.46920000	6.31830000
H	0	4.60080000	5.60040000	4.39410000
H	0	6.16110000	-2.23500000	3.91210000
Al	0	-1.17170000	1.40520000	4.73560000
O	0	-2.78000000	0.96390000	5.57550000
O	0	-0.26240000	2.57450000	5.63390000
O	0	-0.10150000	0.15410000	4.34560000
C	0	-2.96230000	0.13960000	6.74590000
C	0	-3.62680000	-1.16110000	6.35710000
C	0	-0.39440000	3.92910000	5.90640000
C	0	-0.23820000	4.21700000	7.38900000
H	0	-3.54610000	0.71410000	7.47210000
H	0	-1.96880000	-0.04380000	7.16940000
H	0	-4.61100000	-0.98320000	5.91420000
H	0	-3.74280000	-1.79880000	7.23720000
H	0	-3.01220000	-1.69190000	5.62380000
H	0	-1.34990000	4.33710000	5.54430000
H	0	0.46030000	4.44660000	5.37840000
H	0	-1.03390000	3.69780000	7.92980000
H	0	-0.31190000	5.28670000	7.59370000
H	0	0.73110000	3.85470000	7.74140000
C	0	2.08240000	0.55680000	5.61510000
C	0	1.81290000	0.38020000	6.96170000

H	0	1.83910000	1.49010000	5.11160000
H	0	2.46150000	-0.27080000	5.01180000
H	0	2.12560000	-0.52490000	7.47310000
H	0	0.86830000	0.02600000	6.30340000
H	0	1.48180000	1.23870000	7.53830000

$Im3^{B\text{-}OEt}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000
Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76020000	0.00000000	0.74280000

Si	-1	-5.76020000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68030000	0.74280000
Si	-1	1.92000000	7.68020000	0.74280000
Si	-1	1.92000000	3.84010000	0.74280000
Si	-1	1.92000000	0.00000000	0.74280000
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68020000	0.74280000
Si	-1	5.76010000	3.84010000	0.74280000
Si	-1	5.76010000	0.00000000	0.74280000
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000
H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000

H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000
H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05810000	0.00000000	0.02890000
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00474700	5.77685200	2.04218200
Si	0	-5.04479400	1.89705800	1.93928400
Si	0	-4.97056600	-1.93788400	1.98858400
Si	0	-5.04078000	-5.75326000	1.94049900
Si	0	-2.43943000	5.74461600	2.02619100
Si	0	-2.62186500	1.93824200	1.83005500
Si	0	-2.46385000	-1.92112300	1.99772000
Si	0	-2.60587900	-5.74406400	1.93982500
Si	0	2.36279000	5.75571600	1.96063400
Si	0	2.70371100	2.01740400	1.98418400
Si	0	2.38240600	-1.93698600	2.00100800

Si	0	2.60600700	-5.74292900	1.93851000
Si	0	4.82682900	5.65902600	1.97943800
Si	0	5.12174300	1.91683000	1.91928800
Si	0	4.92004500	-1.94362900	2.00294800
Si	0	5.04185800	-5.75412300	1.93893000
O	0	-5.61208200	5.85352000	3.58812900
O	0	-5.17006000	1.77559800	3.60847100
O	0	-5.33155400	-2.06288300	3.62910200
O	0	-5.25547300	-5.61135400	3.60672400
O	0	-1.49662800	5.69525500	3.40830800
O	0	-2.30611400	2.06305700	3.53713300
O	0	-1.66376200	-1.89131100	3.43638400
O	0	-2.39749000	-5.63486400	3.60595200
O	0	1.58067500	5.78904900	3.42684200
O	0	2.66454400	2.60802200	3.56032500
O	0	1.46916600	-2.01519400	3.37208500
O	0	2.40011000	-5.62479000	3.60383000
O	0	4.86651900	4.97502900	3.66588700
O	0	5.42213000	2.16465200	3.53491100
O	0	5.22234700	-2.05214900	3.65249000
O	0	5.25734500	-5.61537000	3.60402100
H	0	-5.25074400	5.25553100	4.25676300
H	0	-6.22317500	-2.34811200	3.85908500
Al	0	-3.80446600	2.01876000	4.63042100
Al	0	-3.82241300	-5.38446500	4.53044500
Cl	0	-3.97460900	3.75557400	5.84273900
Cl	0	-3.87491200	-4.99316500	6.56322400
Al	0	-0.07017400	-1.73689900	4.15130200
Al	0	0.02403100	6.00294900	4.13902500
Cl	0	-0.19479300	-2.55983100	6.11560900
Cl	0	0.00245300	7.34689400	5.74872100
Al	0	3.82698700	-5.34631200	4.51945800
Al	0	4.19443600	3.18851400	4.24208800
Cl	0	3.85610600	-4.87410000	6.53465400
Cl	0	4.05938400	3.71706500	6.29216400
H	0	4.68422400	5.59730700	4.38926800
H	0	6.13344200	-2.12252100	3.95872900
Al	0	-1.15922700	1.39775700	4.77196900

O	0	-2.72543700	0.85546300	5.56252900
O	0	-0.20163200	2.53993400	5.57925200
O	0	0.00018000	0.12111100	4.34895700
C	0	-2.92446800	0.05916900	6.75908200
C	0	-3.68544700	-1.19545000	6.39950100
C	0	-0.15109900	3.89067100	5.90045200
C	0	0.24356000	4.09114800	7.35295900
H	0	-3.44975700	0.68509700	7.48687900
H	0	-1.93292400	-0.18117000	7.15380000
H	0	-4.66620400	-0.95525300	5.97778700
H	0	-3.82395200	-1.81483600	7.28916800
H	0	-3.12408000	-1.77122700	5.65842700
H	0	-1.11465500	4.38793200	5.69874200
H	0	0.66420600	4.33780600	5.26985500
H	0	-0.52694400	3.65647900	7.99438000
H	0	0.34363000	5.15271100	7.58738000
H	0	1.19398700	3.58896700	7.54428600
C	0	3.04752000	0.19391900	5.44009700
C	0	2.70235300	-0.89038000	6.13200700
H	0	2.81197500	1.19341100	5.79795300
H	0	3.60987800	0.10958500	4.51045400
H	0	2.93858200	-1.88855600	5.77661500
H	0	0.91745600	0.37820500	4.58680900
H	0	2.16837600	-0.82224000	7.07514600

$P2^{B\text{-}OEt}$

Atom	**Fix/Relax**	**X**	**Y**	**Z**
Si	-1	-3.84010000	5.76010000	-1.97260000
Si	-1	-3.84010000	1.92000000	-1.97260000
Si	-1	-3.84010000	-1.92000000	-1.97260000
Si	-1	-3.84010000	-5.76010000	-1.97260000
Si	-1	0.00000000	5.76010000	-1.97260000
Si	-1	0.00000000	1.92000000	-1.97260000
Si	-1	0.00000000	-1.92000000	-1.97260000
Si	-1	0.00000000	-5.76010000	-1.97260000
Si	-1	3.84010000	5.76010000	-1.97260000
Si	-1	3.84010000	1.92000000	-1.97260000
Si	-1	3.84010000	-1.92000000	-1.97260000

Si	-1	3.84010000	-5.76010000	-1.97260000
Si	-1	-3.84010000	7.68020000	-0.61490000
Si	-1	-3.84010000	3.84010000	-0.61490000
Si	-1	-3.84010000	0.00000000	-0.61490000
Si	-1	-3.84010000	-3.84010000	-0.61490000
Si	-1	-3.84010000	-7.68020000	-0.61490000
Si	-1	0.00000000	7.68020000	-0.61490000
Si	-1	0.00000000	3.84010000	-0.61490000
Si	-1	0.00000000	0.00000000	-0.61490000
Si	-1	0.00000000	-3.84010000	-0.61490000
Si	-1	0.00000000	-7.68020000	-0.61490000
Si	-1	3.84010000	7.68020000	-0.61490000
Si	-1	3.84010000	3.84010000	-0.61490000
Si	-1	3.84010000	0.00000000	-0.61490000
Si	-1	3.84010000	-3.84010000	-0.61490000
Si	-1	3.84010000	-7.68020000	-0.61490000
Si	-1	-5.76010000	7.68020000	0.74280000
Si	-1	-5.76010000	3.84010000	0.74280000
Si	-1	-5.76020000	0.00000000	0.74280000
Si	-1	-5.76020000	-3.84010000	0.74280000
Si	-1	-5.76010000	-7.68020000	0.74280000
Si	-1	-1.92000000	7.68020000	0.74280000
Si	-1	-1.92000000	3.84010000	0.74280000
Si	-1	-1.92000000	0.00000000	0.74280000
Si	-1	-1.92000000	-3.84010000	0.74280000
Si	-1	-1.92000000	-7.68030000	0.74280000
Si	-1	1.91999900	7.68020100	0.74280000
Si	-1	1.91999900	3.84009900	0.74280000
Si	-1	1.92000000	-0.00000100	0.74280100
Si	-1	1.92000000	-3.84010000	0.74280000
Si	-1	1.92000000	-7.68020000	0.74280000
Si	-1	5.76010000	7.68019900	0.74280000
Si	-1	5.76010200	3.84010300	0.74280000
Si	-1	5.76009900	-0.00000200	0.74280100
Si	-1	5.76010000	-3.84010000	0.74280000
Si	-1	5.76010000	-7.68020000	0.74280000
H	-1	-2.97390000	5.79380000	-3.16220000
H	-1	-5.23870000	5.77270000	-2.51530000

H	-1	-2.98160000	1.92030000	-3.17130000
H	-1	-5.23930000	1.92050000	-2.51900000
H	-1	-2.98150000	-1.92030000	-3.17120000
H	-1	-5.23930000	-1.92050000	-2.51900000
H	-1	-2.97400000	-5.79360000	-3.16220000
H	-1	-5.23870000	-5.77270000	-2.51530000
H	-1	1.16760000	5.71010000	-2.86270000
H	-1	-1.16750000	5.71010000	-2.86280000
H	-1	1.17310000	1.91760000	-2.85730000
H	-1	-1.17330000	1.91760000	-2.85710000
H	-1	1.17330000	-1.91760000	-2.85710000
H	-1	-1.17310000	-1.91760000	-2.85730000
H	-1	1.16750000	-5.71010000	-2.86280000
H	-1	-1.16760000	-5.71010000	-2.86270000
H	-1	5.23870000	5.77270000	-2.51530000
H	-1	2.97400000	5.79360000	-3.16220000
H	-1	5.23930000	1.92050000	-2.51900000
H	-1	2.98150000	1.92030000	-3.17120000
H	-1	5.23930000	-1.92050000	-2.51900000
H	-1	2.98160000	-1.92030000	-3.17130000
H	-1	5.23870000	-5.77270000	-2.51530000
H	-1	2.97390000	-5.79380000	-3.16220000
H	-1	-3.82400000	8.85870000	-1.53420000
H	-1	-3.82400000	-8.85870000	-1.53420000
H	-1	0.00000000	8.92610000	-1.42910000
H	-1	0.00000000	-8.92610000	-1.42910000
H	-1	3.82400000	8.85870000	-1.53420000
H	-1	3.82400000	-8.85870000	-1.53420000
H	-1	-7.00580000	7.40190000	-0.01410000
H	-1	-5.87800000	8.93300000	1.52980000
H	-1	-7.05960000	3.84790000	0.03190000
H	-1	-7.05810000	0.00000000	0.02890000
H	-1	-7.05950000	-3.84760000	0.03180000
H	-1	-5.87620000	-8.93250000	1.53080000
H	-1	-7.00650000	-7.40340000	-0.01330000
H	-1	-1.90150000	8.88670000	1.61890000
H	-1	-1.90150000	-8.88670000	1.61880000
H	-1	1.90150000	8.88670000	1.61880000

H	-1	1.90150000	-8.88670000	1.61890000
H	-1	5.87620000	8.93250000	1.53080000
H	-1	7.00650000	7.40340000	-0.01330000
H	-1	7.05950000	3.84760000	0.03180000
H	-1	7.05809900	0.00000000	0.02889900
H	-1	7.05960000	-3.84790000	0.03190000
H	-1	7.00580000	-7.40190000	-0.01410000
H	-1	5.87800000	-8.93300000	1.52980000
Si	0	-5.00485100	5.77696100	2.04199500
Si	0	-5.05667300	1.89871200	1.93177200
Si	0	-4.95557200	-1.93798500	1.99751300
Si	0	-5.04380400	-5.75392900	1.93917000
Si	0	-2.43973700	5.74453400	2.02640400
Si	0	-2.63894900	1.94621900	1.81974500
Si	0	-2.42888800	-1.91545600	2.01374900
Si	0	-2.60817600	-5.74384100	1.94053500
Si	0	2.35401000	5.75500800	1.95984300
Si	0	2.68365300	1.97808800	1.94486000
Si	0	2.42250800	-1.92537800	2.00104100
Si	0	2.60714400	-5.74561000	1.93918900
Si	0	4.80480000	5.63527300	1.99816100
Si	0	5.10606800	1.91638200	1.91076600
Si	0	4.94850600	-1.93961500	1.99933200
Si	0	5.04169700	-5.75569400	1.94000500
O	0	-5.61445100	5.85703400	3.58703600
O	0	-5.19128200	1.78842300	3.60103000
O	0	-5.32280600	-2.07012600	3.63648700
O	0	-5.26362400	-5.61169700	3.60528100
O	0	-1.49860400	5.69873500	3.40922200
O	0	-2.35111600	2.15666100	3.52041900
O	0	-1.57831300	-1.85642200	3.43031400
O	0	-2.40416700	-5.62596800	3.60747300
O	0	1.57670900	5.75576500	3.43030400
O	0	1.54585800	-1.90943900	3.40039500
O	0	2.39961400	-5.65732500	3.60534300
O	0	5.29261000	-2.04707700	3.63529500
O	0	5.25562500	-5.64437300	3.60648000
H	0	-5.26218000	5.25707600	4.25842000

H	0	-6.22016300	-2.34060000	3.86241800
Al	0	-3.82918100	2.05362600	4.62080500
Al	0	-3.83219600	-5.36610700	4.52472200
Cl	0	-4.03781700	3.74785100	5.88531800
Cl	0	-3.86628300	-4.92214800	6.54735300
Al	0	0.00389300	-1.49399900	4.09853600
Al	0	0.02196600	6.01089800	4.14086900
Cl	0	-0.06633600	-1.80519000	6.20940200
Cl	0	0.01690700	7.42698000	5.68922500
Al	0	3.82585100	-5.45713600	4.54297900
Cl	0	3.85065600	-5.19578300	6.59416100
H	0	6.20940700	-2.16047500	3.90815300
Al	0	-1.16817300	1.50364200	4.72171300
O	0	-2.70673800	0.90065200	5.52573200
O	0	-0.22679700	2.65180800	5.53620400
O	0	0.02112100	0.38861100	3.98847000
C	0	-2.94989600	0.17840200	6.76424300
C	0	-3.64077500	-1.12536200	6.43897800
C	0	-0.22840500	3.98568700	5.91711600
C	0	0.04162900	4.14589000	7.40260900
H	0	-3.55048100	0.83098700	7.40603300
H	0	-1.98117800	0.01120700	7.23896700
H	0	-4.60030600	-0.95219700	5.94208900
H	0	-3.81505600	-1.69522400	7.35507600
H	0	-3.01164100	-1.72164400	5.77298400
H	0	-1.17791700	4.48117200	5.65284500
H	0	0.63604700	4.46615500	5.38106100
H	0	-0.77036700	3.67529100	7.96256200
H	0	0.09580500	5.20191700	7.67563000
H	0	0.98289800	3.65472000	7.65606700
H	0	0.91155400	0.79398700	4.05503100
O	0	2.57353900	2.39130100	3.57402000
O	0	4.74691900	4.88829000	3.67020200
O	0	5.36755200	2.12923600	3.53671200
Al	0	4.08208900	3.06763200	4.25437200
Cl	0	3.88662300	3.59301900	6.29206300
H	0	4.52438000	5.50135400	4.39062800

Table S2. The interfacial interaction energies, $E_{\text{interface}}$, between $\sigma^*_{\text{C-H}}$ and other orbitals of the transition state (TS) and the corresponding imtermediate (Im) of alkyl halide (R-Cl) elimination on the surface.

Donor NBO (i)	Acceptor NBO (j)	$E_{\text{interface}}$ (kcal/mol)
$Im1^{B\text{-}OEt}$		
BD(1)Si102-O118	BD*(1)C143-H152	0.06
BD(1)Si106-O121	BD*(1)C143-H152	0.05
LP(1)O114	BD*(1)C143-H150	0.58
LP(2)O114	BD*(1)C143-H150	0.08
LP(1)O118	BD*(1)C143-H152	0.36
LP(2)O118	BD*(1)C143-H152	0.06
LP(3)O118	BD*(1)C143-H152	0.14
LP(2)O121	BD*(1)C143-H152	0.06
LP(3)O121	BD*(1)C143-H152	0.10
LP*(1)Al128	BD*(1)C143-H152	0.06
LP(1)Cl130	BD*(1)C143-H151	0.06
LP(3)Cl130	BD*(1)C143-H151	0.12
BD(1)Si104-O120	BD*(1)C144-H153	0.06
BD(1)Si104-O120	BD*(1)C144-H154	0.11
LP(1)O116	BD*(1)C144-H153	0.33
LP(2)O116	BD*(1)C144-H153	0.15
LP(2)O116	BD*(1)C144-H154	0.13
LP(2)O120	BD*(1)C144-H154	0.83
LP(3)O120	BD*(1)C144-H153	0.07
LP(3)O120	BD*(1)C144-H154	0.07
BD(1)Si102-O118	BD*(1)C146-H159	0.05
LP(1)O118	BD*(1)C146-H159	0.05
LP(3)O118	BD*(1)C146-H159	0.09
LP(1)O121	BD*(1)C146-H159	0.06
LP(2)O121	BD*(1)C146-H159	0.77
LP(3)O121	BD*(1)C146-H159	0.07
LP(1)O163	BD*(1)C146-H158	1.30
LP(2)O163	BD*(1)C146-H158	1.53
LP(3)O163	BD*(1)C146-H158	0.30
LP*(1)Al127	BD*(1)C143-H150	0.30
LP*(1)Al127	BD*(1)C143-H151	0.09
LP*(2)Al127	BD*(1)C142-H148	0.50

LP*(3)Al127	BD*(1)C142-H148	0.26
LP*(3)Al127	BD*(1)C142-H149	0.10
LP*(3)Al127	BD*(1)C143-H150	0.33
LP*(1)Al127	BD*(1)C144-H153	0.11
LP(1)Cl129	BD*(1)C144-H153	0.16
LP(2)Cl129	BD*(1)C144-H153	0.94
LP(2)Cl129	BD*(1)C144-H154	0.09
LP(3)Cl129	BD*(1)C144-H153	0.36
LP*(1)Al127	BD*(1)C147-H161	0.05
LP*(1)Al131	BD*(1)C143-H152	0.11
LP*(2)Al131	BD*(1)C143-H152	0.35
LP*(3)Al131	BD*(1)C143-H152	1.08
LP(2)Cl133	BD*(1)C143-H152	0.20
BD(1)Al131-Cl133	BD*(1)C146-H158	0.06
LP*(1)Al131	BD*(1)C147-H160	0.15
LP*(2)Al131	BD*(1)C147-H160	0.06
LP*(3)Al131	BD*(1)C146-H158	0.41
LP*(3)Al131	BD*(1)C146-H159	2.06
LP*(3)Al131	BD*(1)C147-H160	0.09
LP(1)Cl133	BD*(1)C147-H160	0.10
LP(2)Cl133	BD*(1)C147-H160	0.05
LP(3)Cl133	BD*(1)C146-H158	0.05
LP(3)Cl133	BD*(1)C147-H160	1.48
BD(1)Al132-Cl134	BD*(1)C144-H154	0.22
CR(1)Al132	BD*(1)C144-H154	0.05
CR(2)Al132	BD*(1)C144-H154	0.37
CR(3)Al132	BD*(1)C144-H154	0.06
LP*(1)Al132	BD*(1)C144-H153	0.09
LP*(1)Al132	BD*(1)C144-H154	1.27
LP*(1)Al132	BD*(1)C145-H155	0.05
LP*(1)Al132	BD*(1)C145-H156	0.07
LP*(2)Al132	BD*(1)C144-H154	5.01
LP*(2)Al132	BD*(1)C145-H156	0.12
LP*(3)Al132	BD*(1)C144-H153	1.77
LP*(3)Al132	BD*(1)C144-H154	0.97
LP(1)Cl134	BD*(1)C145-H156	0.08
LP(3)Cl134	BD*(1)C144-H154	0.05
LP(3)Cl134	BD*(1)C145-H156	0.94

LP*(1)Al138	BD*(1)C142-H149	0.23
LP*(2)Al138	BD*(1)C142-H149	0.49
LP*(3)Al138	BD*(1)C142-H148	0.16
LP*(3)Al138	BD*(1)C142-H149	0.42
LP*(3)Al138	BD*(1)C143-H152	0.10
LP*(4)Al138	BD*(1)C142-H149	0.21
LP*(4)Al138	BD*(1)C143-H151	0.07
LP*(1)Al138	BD*(1)C144-H153	0.07
LP*(2)Al138	BD*(1)C145-H155	0.17
LP*(3)Al138	BD*(1)C144-H153	0.50
LP*(3)Al138	BD*(1)C144-H154	0.10
LP*(3)Al138	BD*(1)C145-H155	0.06
LP*(4)Al138	BD*(1)C145-H155	0.08
LP*(4)Al138	BD*(1)C145-H156	0.07
LP*(4)Al138	BD*(1)C145-H157	0.10
LP*(1)Al138	BD*(1)C147-H161	0.23
LP*(2)Al138	BD*(1)C146-H158	0.25
LP*(2)Al138	BD*(1)C147-H161	0.34
LP*(2)Al138	BD*(1)C147-H162	0.06
LP*(3)Al138	BD*(1)C147-H162	0.19
LP*(4)Al138	BD*(1)C146-H158	0.87
LP*(4)Al138	BD*(1)C146-H159	0.46
LP*(4)Al138	BD*(1)C147-H160	0.10
LP*(4)Al138	BD*(1)C147-H161	1.69
LP*(4)Al138	BD*(1)C147-H162	0.33
LP(1)O139	BD*(1)C142-H148	3.49
LP(1)O139	BD*(1)C143-H151	0.71
LP(2)O139	BD*(1)C142-H148	1.67
LP(2)O139	BD*(1)C142-H149	4.72
LP(1)O140	BD*(1)C144-H153	8.22
LP(1)O140	BD*(1)C144-H154	1.17
LP(2)O140	BD*(1)C144-H154	7.41
LP(2)O140	BD*(1)C145-H156	0.59
LP(3)O140	BD*(1)C144-H153	0.69
LP(3)O140	BD*(1)C144-H154	0.64
LP(1)O140	BD*(1)C146-H158	0.21
LP(1)O140	BD*(1)C146-H159	0.57
LP(1)O140	BD*(1)C147-H161	0.29

LP(2)O140	BD*(1)C146-H158	0.15
LP(2)O140	BD*(1)C147-H161	0.41
LP(1)O141	BD*(1)C146-H158	2.05
LP(1)O141	BD*(1)C147-H162	0.62
LP(2)O141	BD*(1)C146-H158	1.97
LP(2)O141	BD*(1)C146-H159	4.03
LP*(1)Al166	BD*(1)C145-H157	0.09
LP*(2)Al166	BD*(1)C144-H154	0.12
LP*(3)Al166	BD*(1)C144-H154	0.19
LP(1)Cl167	BD*(1)C145-H157	0.09
LP(2)Cl167	BD*(1)C145-H157	0.38
LP(3)Cl167	BD*(1)C145-H157	0.06
LP*(3)Al166	BD*(1)C146-H158	0.81
Total		77.1
$TS1^{B\text{-}OEt}$		
BD(1)Si102-O118	BD*(1)C148-H155	0.06
LP(1)O114	BD*(1)C148-H153	0.61
LP(2)O114	BD*(1)C148-H153	0.05
LP(1)O118	BD*(1)C148-H155	0.07
LP(2)O118	BD*(1)C148-H155	0.32
LP(3)O118	BD*(1)C148-H155	0.18
BD(1)Si104-O120	BD*(1)C149-H157	0.14
LP(1)O116	BD*(1)C149-H156	0.08
LP(2)O116	BD*(1)C149-H157	0.09
LP(2)O120	BD*(1)C149-H157	0.61
LP(3)O120	BD*(1)C149-H156	0.07
LP*(1)Al138	BD*(1)C149-H156	0.05
LP*(1)Al138	BD*(1)C149-H157	0.21
LP*(1)Al138	BD*(1)C150-H160	0.10
LP(1)Cl140	BD*(1)C150-H160	0.15
LP(2)Cl140	BD*(1)C150-H160	0.61
LP(3)Cl140	BD*(1)C150-H160	0.10
BD*(1)O121-Al138	BD*(1)C149-H157	0.05
BD(1)Si101-O117	BD*(1)C163-H168	0.07
BD(1)Si102-O118	BD*(1)C162-H164	0.07
LP(2)O117	BD*(1)C163-H168	0.06
LP(3)O118	BD*(1)C162-H164	0.09
LP(2)O122	BD*(1)C162-H164	0.38

LP*(2)Al138	BD*(1)C162-H164	0.16
LP*(2)Al138	BD*(1)C163-H166	0.09
LP(1)Cl139	BD*(1)C162-H165	0.10
LP(2)Cl139	BD*(1)C162-H165	0.08
LP(3)Cl139	BD*(1)C162-H165	0.48
LP(2)Cl140	BD*(1)C163-H166	0.15
LP(3)Cl140	BD*(1)C163-H166	0.10
LP*(1)Al130	BD*(1)C148-H153	0.22
LP*(1)Al130	BD*(1)C148-H154	0.06
LP*(2)Al130	BD*(1)C147-H151	0.68
LP*(3)Al130	BD*(1)C147-H151	0.31
LP*(3)Al130	BD*(1)C147-H152	0.16
LP*(3)Al130	BD*(1)C148-H153	0.31
LP(3)Cl132	BD*(1)C147-H151	0.05
LP*(1)Al130	BD*(1)C149-H156	0.12
LP(1)Cl132	BD*(1)C149-H156	0.07
LP(2)Cl132	BD*(1)C149-H156	0.71
LP(3)Cl132	BD*(1)C149-H156	0.17
LP*(1)Al134	BD*(1)C148-H155	0.08
LP*(2)Al134	BD*(1)C148-H155	0.34
LP*(3)Al134	BD*(1)C148-H155	0.12
LP*(4)Al134	BD*(1)C148-H155	1.23
LP*(1)Al134	BD*(1)C162-H164	0.47
LP*(2)Al134	BD*(1)C162-H164	0.39
LP*(2)Al134	BD*(1)C162-H165	0.18
LP*(4)Al134	BD*(1)C162-H164	2.50
LP*(4)Al134	BD*(1)C162-H165	0.29
BD(1)Al135-Cl136	BD*(1)C149-H157	0.25
CR(1)Al135	BD*(1)C149-H157	0.07
CR(2)Al135	BD*(1)C149-H157	0.54
CR(3)Al135	BD*(1)C149-H157	0.10
LP*(1)Al135	BD*(1)C149-H156	0.11
LP*(1)Al135	BD*(1)C149-H157	3.20
LP*(1)Al135	BD*(1)C150-H159	0.07
LP*(2)Al135	BD*(1)C149-H157	4.65
LP*(2)Al135	BD*(1)C150-H159	0.14
LP*(3)Al135	BD*(1)C149-H156	1.17
LP*(3)Al135	BD*(1)C149-H157	1.22

LP(1)Cl136	BD*(1)C150-H159	0.11
LP(3)Cl136	BD*(1)C149-H157	0.10
LP(3)Cl136	BD*(1)C150-H159	1.11
LP*(1)Al143	BD*(1)C147-H152	0.11
LP*(2)Al143	BD*(1)C147-H152	0.28
LP*(3)Al143	BD*(1)C147-H151	0.08
LP*(3)Al143	BD*(1)C147-H152	1.00
LP(1)O146	BD*(1)C148-H155	0.05
LP(2)O146	BD*(1)C147-H152	0.07
LP*(1)Al143	BD*(1)C149-H156	0.43
LP*(2)Al143	BD*(1)C149-H157	0.19
LP*(3)Al143	BD*(1)C149-H157	0.05
LP*(3)Al143	BD*(1)C150-H158	0.11
BD*(1)Al143-O146	BD*(1)C149-H156	0.14
LP*(1)Al143	BD*(1)C162-H164	0.08
LP*(2)Al143	BD*(1)C163-H168	0.15
LP*(3)Al143	BD*(1)C162-H165	0.07
LP*(3)Al143	BD*(1)C163-H166	0.09
LP*(3)Al143	BD*(1)C163-H167	0.06
LP*(3)Al143	BD*(1)C163-H168	2.36
LP(2)O146	BD*(1)C162-H164	0.10
LP(2)O146	BD*(1)C162-H165	0.06
LP(1)O144	BD*(1)C147-H151	2.92
LP(1)O144	BD*(1)C147-H152	0.61
LP(1)O144	BD*(1)C148-H154	0.84
LP(2)O144	BD*(1)C147-H151	2.64
LP(2)O144	BD*(1)C147-H152	4.89
LP(1)O145	BD*(1)C149-H156	7.91
LP(2)O145	BD*(1)C149-H156	1.15
LP(2)O145	BD*(1)C149-H157	10.47
LP(1)O145	BD*(1)C163-H168	1.98
LP(2)O145	BD*(1)C163-H168	0.31
LP(3)O145	BD*(1)C163-H168	0.06
LP(2)Cl161	BD*(1)C147-H151	0.05
LP(2)Cl161	BD*(1)C147-H152	0.31
LP(2)Cl161	BD*(1)C148-H155	0.05
LP(1)Cl161	BD*(1)C162-H164	1.09
LP(2)Cl161	BD*(1)C162-H165	1.44

LP(2)Cl161	BD*(1)C163-H166	0.70
LP(3)Cl161	BD*(1)C162-H164	1.45
Total		71.0
$Im1^{B\text{-}OiPr}$		
LP(1)O114	BD*(1)C143-H150	0.06
LP(1)O118	BD*(1)C143-H150	0.50
LP(3)O118	BD*(1)C143-H150	0.08
LP*(1)Al128	BD*(1)C143-H150	0.15
LP(1)Cl130	BD*(1)C143-H151	0.09
LP(3)Cl130	BD*(1)C143-H151	0.17
LP(1)O116	BD*(1)C144-H153	0.26
LP(2)O116	BD*(1)C144-H153	0.33
LP(2)O116	BD*(1)C154-H171	0.06
LP(1)O120	BD*(1)C154-H169	0.26
LP(1)O120	BD*(1)C154-H171	0.08
LP(2)O120	BD*(1)C154-H169	0.20
LP(1)O172	BD*(1)C154-H169	0.45
LP(2)O172	BD*(1)C154-H169	0.08
BD(1)Si24-Si39	BD*(1)C159-H166	0.08
BD(1)Si102-O118	BD*(1)C159-H167	0.07
BD(1)Si106-Si110	BD*(1)C159-H166	0.06
LP(3)O118	BD*(1)C159-H167	0.11
LP(1)O121	BD*(1)C159-H166	0.05
LP(1)O121	BD*(1)C159-H168	0.33
LP(2)O121	BD*(1)C159-H168	0.29
LP(3)O121	BD*(1)C159-H167	0.07
LP(1)O172	BD*(1)C146-H158	0.22
LP(2)O172	BD*(1)C146-H158	0.09
LP(2)O172	BD*(1)C159-H166	0.12
LP(2)O172	BD*(1)C159-H167	0.09
LP(2)O172	BD*(1)C159-H168	0.07
LP(3)O172	BD*(1)C146-H158	0.07
LP(3)O172	BD*(1)C159-H166	0.09
BD(1)Al127-Cl129	BD*(1)C149-H164	0.06
LP*(1)Al127	BD*(1)C142-H148	0.35
LP*(1)Al127	BD*(1)C149-H164	0.17
LP*(2)Al127	BD*(1)C149-H163	0.16
LP*(2)Al127	BD*(1)C149-H164	0.23

LP*(3)Al127	BD*(1)C142-H148	0.54
LP*(3)Al127	BD*(1)C149-H164	0.34
LP(3)Cl129	BD*(1)C142-H148	0.08
LP(3)Cl129	BD*(1)C149-H164	0.73
BD(1)Al127-Cl129	BD*(1)C144-H153	0.07
LP*(1)Al127	BD*(1)C144-H153	0.29
LP*(1)Al127	BD*(1)C145-H155	0.09
LP*(3)Al127	BD*(1)C144-H153	0.13
LP(1)Cl129	BD*(1)C144-H153	0.10
LP(1)Cl129	BD*(1)C145-H155	0.17
LP(2)Cl129	BD*(1)C144-H153	0.81
LP(2)Cl129	BD*(1)C145-H155	0.35
LP(2)Cl129	BD*(1)C145-H157	0.11
LP(3)Cl129	BD*(1)C144-H153	0.58
LP(3)Cl129	BD*(1)C145-H155	0.14
LP*(1)Al127	BD*(1)C146-H158	0.16
LP*(1)Al127	BD*(1)C147-H161	0.10
LP*(1)Al131	BD*(1)C143-H152	0.14
LP*(2)Al131	BD*(1)C143-H152	0.15
LP*(3)Al131	BD*(1)C143-H150	0.95
LP*(3)Al131	BD*(1)C143-H151	0.14
LP(2)Cl133	BD*(1)C143-H152	0.17
LP(3)Cl133	BD*(1)C143-H152	0.16
LP*(1)Al131	BD*(1)C147-H160	0.21
LP*(1)Al131	BD*(1)C159-H167	0.17
LP*(2)Al131	BD*(1)C146-H158	0.06
LP*(2)Al131	BD*(1)C147-H160	0.16
LP*(2)Al131	BD*(1)C147-H162	0.05
LP*(2)Al131	BD*(1)C159-H167	0.06
LP*(2)Al131	BD*(1)C159-H168	0.10
LP*(3)Al131	BD*(1)C146-H158	0.08
LP*(3)Al131	BD*(1)C147-H160	0.09
LP*(3)Al131	BD*(1)C159-H166	0.07
LP*(3)Al131	BD*(1)C159-H167	1.68
LP*(3)Al131	BD*(1)C159-H168	0.73
LP(1)Cl133	BD*(1)C147-H160	0.06
LP(3)Cl133	BD*(1)C147-H160	1.34
LP(3)Cl133	BD*(1)C159-H167	0.06

BD(1)Al132-Cl134	BD*(1)C154-H170	0.11
BD(1)Al132-Cl134	BD*(1)C154-H171	2.18
CR(2)Al132	BD*(1)C154-H170	0.25
CR(2)Al132	BD*(1)C154-H171	0.20
CR(3)Al132	BD*(1)C154-H170	0.06
CR(5)Al132	BD*(1)C154-H171	0.09
LP*(1)Al132	BD*(1)C144-H153	0.11
LP*(1)Al132	BD*(1)C145-H156	0.07
LP*(1)Al132	BD*(1)C154-H169	1.35
LP*(1)Al132	BD*(1)C154-H170	0.71
LP*(1)Al132	BD*(1)C154-H171	0.77
LP*(2)Al132	BD*(1)C144-H153	0.91
LP*(2)Al132	BD*(1)C145-H156	0.16
LP*(2)Al132	BD*(1)C154-H170	0.97
LP*(2)Al132	BD*(1)C154-H171	0.09
LP*(3)Al132	BD*(1)C144-H153	0.09
LP*(3)Al132	BD*(1)C154-H169	0.11
LP*(3)Al132	BD*(1)C154-H170	1.05
LP*(3)Al132	BD*(1)C154-H171	2.48
LP(1)Cl134	BD*(1)C154-H169	0.16
LP(1)Cl134	BD*(1)C154-H171	0.07
LP(3)Cl134	BD*(1)C154-H171	1.45
LP*(1)Al138	BD*(1)C143-H151	0.07
LP*(1)Al138	BD*(1)C143-H152	0.11
LP*(1)Al138	BD*(1)C149-H165	0.16
LP*(2)Al138	BD*(1)C142-H148	0.10
LP*(2)Al138	BD*(1)C143-H151	0.14
LP*(2)Al138	BD*(1)C143-H152	0.32
LP*(2)Al138	BD*(1)C149-H163	0.19
LP*(2)Al138	BD*(1)C149-H165	0.71
LP*(3)Al138	BD*(1)C143-H151	0.32
LP*(3)Al138	BD*(1)C143-H152	0.58
LP*(3)Al138	BD*(1)C149-H163	0.05
LP*(4)Al138	BD*(1)C143-H152	0.66
LP*(4)Al138	BD*(1)C149-H165	0.59
LP*(1)Al138	BD*(1)C144-H153	0.08
LP*(2)Al138	BD*(1)C145-H155	0.06
LP*(2)Al138	BD*(1)C154-H169	0.29

LP*(3)Al138	BD*(1)C144-H153	0.87
LP*(3)Al138	BD*(1)C145-H155	0.13
LP*(3)Al138	BD*(1)C145-H156	0.05
LP*(3)Al138	BD*(1)C154-H169	0.40
LP*(3)Al138	BD*(1)C154-H171	0.07
LP*(4)Al138	BD*(1)C144-H153	0.12
LP*(4)Al138	BD*(1)C145-H156	0.06
LP*(4)Al138	BD*(1)C145-H157	0.09
LP*(4)Al138	BD*(1)C154-H169	0.10
LP*(4)Al138	BD*(1)C154-H170	0.14
LP*(4)Al138	BD*(1)C154-H171	0.18
LP*(1)Al138	BD*(1)C146-H158	0.12
LP*(1)Al138	BD*(1)C147-H161	0.27
LP*(2)Al138	BD*(1)C146-H158	0.38
LP*(2)Al138	BD*(1)C147-H161	0.43
LP*(3)Al138	BD*(1)C147-H162	0.13
LP*(3)Al138	BD*(1)C159-H167	0.05
LP*(4)Al138	BD*(1)C146-H158	1.67
LP*(4)Al138	BD*(1)C147-H160	0.16
LP*(4)Al138	BD*(1)C147-H161	1.94
LP*(4)Al138	BD*(1)C147-H162	0.36
LP(1)O139	BD*(1)C142-H148	1.70
LP(1)O139	BD*(1)C149-H163	0.72
LP(2)O139	BD*(1)C142-H148	3.09
LP(1)O140	BD*(1)C143-H152	0.05
LP(2)O140	BD*(1)C149-H165	0.14
LP(3)O140	BD*(1)C149-H165	0.08
LP(1)O140	BD*(1)C144-H153	7.68
LP(2)O140	BD*(1)C145-H156	0.63
LP(2)O140	BD*(1)C154-H171	1.08
LP(3)O140	BD*(1)C144-H153	0.77
LP(1)O140	BD*(1)C146-H158	0.17
LP(1)O140	BD*(1)C147-H160	0.10
LP(1)O140	BD*(1)C147-H161	0.52
LP(2)O140	BD*(1)C146-H158	0.49
LP(2)O140	BD*(1)C147-H161	0.14
LP(1)O141	BD*(1)C143-H152	0.06
LP(3)O141	BD*(1)C143-H152	0.06

LP(1)O141	BD*(1)C146-H158	1.17
LP(1)O141	BD*(1)C147-H162	0.74
LP(2)O141	BD*(1)C146-H158	2.74
LP*(1)Al175	BD*(1)C154-H170	0.27
LP*(3)Al175	BD*(1)C154-H169	0.10
LP*(3)Al175	BD*(1)C154-H170	0.11
LP(1)Cl176	BD*(1)C154-H170	0.08
LP(2)Cl176	BD*(1)C154-H170	1.00
LP(3)Cl176	BD*(1)C154-H170	0.41
LP*(1)Al175	BD*(1)C159-H168	0.15
LP*(2)Al175	BD*(1)C159-H166	0.09
LP*(2)Al175	BD*(1)C159-H167	0.12
LP*(2)Al175	BD*(1)C159-H168	0.43
LP*(3)Al175	BD*(1)C146-H158	0.42
LP*(3)Al175	BD*(1)C159-H167	0.11
LP*(3)Al175	BD*(1)C159-H168	0.08
Total		68.1
$TS1^{B\text{-}OiPr}$		
LP(1)O116	BD*(1)C137-H139	0.12
LP(2)O116	BD*(1)C137-H139	0.09
LP(2)O116	BD*(1)C140-H146	0.06
LP(1)O120	BD*(1)C140-H144	0.34
LP(1)O120	BD*(1)C140-H145	0.06
LP(1)O120	BD*(1)C140-H146	0.12
LP(2)O120	BD*(1)C140-H144	0.25
LP(1)O147	BD*(1)C140-H144	0.28
LP(2)O147	BD*(1)C140-H144	0.05
BD(1)Si101-O117	BD*(1)C155-H157	0.05
LP(1)O114	BD*(1)C156-H159	4.07
LP(3)O117	BD*(1)C155-H157	0.06
LP(3)O118	BD*(1)C156-H161	0.06
LP(3)Cl130	BD*(1)C156-H160	0.10
BD(1)Si102-O118	BD*(1)C171-H175	0.07
BD(1)Si106-O121	BD*(1)C171-H175	0.14
BD(1)Si109-O149	BD*(1)C171-H177	0.06
LP(2)O118	BD*(1)C171-H175	0.06
LP(3)O118	BD*(1)C171-H175	0.07
LP(1)O121	BD*(1)C171-H175	0.44

LP(2)O121	BD*(1)C171-H175	4.65
LP(3)O121	BD*(1)C171-H175	0.80
LP(1)O147	BD*(1)C168-H170	0.87
LP(2)O147	BD*(1)C168-H170	0.62
LP(2)O147	BD*(1)C171-H177	0.05
LP(3)O147	BD*(1)C168-H170	0.28
LP(3)O147	BD*(1)C171-H177	0.08
LP(2)O148	BD*(1)C171-H177	0.07
LP(2)O149	BD*(1)C171-H177	0.48
BD(1)Al127-Cl129	BD*(1)C137-H139	0.07
LP*(1)Al127	BD*(1)C137-H139	0.28
LP*(1)Al127	BD*(1)C138-H141	0.07
LP*(3)Al127	BD*(1)C137-H139	0.16
LP(1)Cl129	BD*(1)C137-H139	0.05
LP(1)Cl129	BD*(1)C138-H141	0.06
LP(2)Cl129	BD*(1)C137-H139	0.80
LP(2)Cl129	BD*(1)C138-H141	0.30
LP(2)Cl129	BD*(1)C138-H143	0.08
LP(3)Cl129	BD*(1)C137-H139	0.53
LP(3)Cl129	BD*(1)C138-H141	0.06
LP*(1)Al127	BD*(1)C156-H159	0.11
LP*(2)Al127	BD*(1)C155-H157	0.35
LP*(2)Al127	BD*(1)C158-H163	0.17
LP*(3)Al127	BD*(1)C155-H157	1.10
LP*(3)Al127	BD*(1)C156-H159	0.09
BD(1)Al127-Cl129	BD*(1)C168-H170	0.06
LP*(1)Al127	BD*(1)C168-H170	0.16
LP*(1)Al127	BD*(1)C169-H173	0.07
LP*(2)Al127	BD*(1)C168-H170	0.11
BD(1)Al131-Cl132	BD*(1)C140-H145	0.08
BD(1)Al131-Cl132	BD*(1)C140-H146	2.08
CR(2)Al131	BD*(1)C140-H145	0.23
CR(2)Al131	BD*(1)C140-H146	0.17
CR(3)Al131	BD*(1)C140-H145	0.06
CR(5)Al131	BD*(1)C140-H146	0.08
LP*(1)Al131	BD*(1)C137-H139	0.10
LP*(1)Al131	BD*(1)C140-H144	1.74
LP*(1)Al131	BD*(1)C140-H145	0.63

LP*(1)Al131	BD*(1)C140-H146	0.88
LP*(2)Al131	BD*(1)C137-H139	0.83
LP*(2)Al131	BD*(1)C138-H142	0.08
LP*(2)Al131	BD*(1)C140-H145	0.84
LP*(2)Al131	BD*(1)C140-H146	0.08
LP*(3)Al131	BD*(1)C137-H139	0.17
LP*(3)Al131	BD*(1)C140-H144	0.12
LP*(3)Al131	BD*(1)C140-H145	1.06
LP*(3)Al131	BD*(1)C140-H146	2.28
LP(1)Cl132	BD*(1)C140-H144	0.19
LP(1)Cl132	BD*(1)C140-H146	0.07
LP(3)Cl132	BD*(1)C140-H146	1.43
LP(1)O136	BD*(1)C137-H139	7.26
LP(2)O136	BD*(1)C138-H142	0.57
LP(2)O136	BD*(1)C140-H146	1.35
LP(3)O136	BD*(1)C137-H139	1.15
LP(2)O136	BD*(1)C158-H162	0.19
LP(2)O136	BD*(1)C158-H163	0.10
LP(1)O136	BD*(1)C168-H170	0.07
LP(1)O136	BD*(1)C169-H172	0.18
LP(1)O136	BD*(1)C169-H173	1.99
LP(2)O136	BD*(1)C168-H170	0.24
LP(2)O136	BD*(1)C169-H173	0.19
BD(1)Al150-Cl151	BD*(1)C140-H145	0.06
LP*(1)Al150	BD*(1)C140-H145	0.31
LP*(2)Al150	BD*(1)C140-H145	0.09
LP*(3)Al150	BD*(1)C140-H144	0.07
LP*(3)Al150	BD*(1)C140-H145	0.23
LP(2)Cl151	BD*(1)C140-H145	1.40
LP(3)Cl151	BD*(1)C140-H145	0.23
LP*(1)Al150	BD*(1)C169-H174	0.27
LP*(2)Al150	BD*(1)C171-H175	0.29
LP*(2)Al150	BD*(1)C171-H177	1.91
LP*(3)Al150	BD*(1)C168-H170	0.11
LP*(3)Al150	BD*(1)C171-H177	0.25
LP(1)Cl151	BD*(1)C169-H174	0.38
LP(2)Cl151	BD*(1)C169-H174	1.43
LP(3)Cl151	BD*(1)C169-H174	0.63

LP(3)Cl151	BD*(1)C171-H177	0.10
LP*(1)Al153	BD*(1)C137-H139	1.36
LP*(1)Al153	BD*(1)C138-H141	0.10
LP*(1)Al153	BD*(1)C140-H144	0.19
LP*(2)Al153	BD*(1)C140-H144	1.04
LP*(2)Al153	BD*(1)C140-H145	0.06
LP*(2)Al153	BD*(1)C140-H146	0.18
LP*(3)Al153	BD*(1)C138-H142	0.07
LP*(3)Al153	BD*(1)C138-H143	0.07
LP*(3)Al153	BD*(1)C140-H145	0.09
LP*(3)Al153	BD*(1)C140-H146	0.15
LP(1)O166	BD*(1)C140-H144	0.06
BD*(1)Al153-O166	BD*(1)C137-H139	0.27
LP*(1)Al153	BD*(1)C158-H162	0.19
LP*(1)Al153	BD*(1)C158-H163	0.27
LP*(2)Al153	BD*(1)C156-H160	0.10
LP*(2)Al153	BD*(1)C156-H161	0.08
LP*(2)Al153	BD*(1)C158-H162	0.22
LP*(2)Al153	BD*(1)C158-H163	0.09
LP*(2)Al153	BD*(1)C158-H164	0.30
LP*(3)Al153	BD*(1)C158-H162	0.48
LP*(3)Al153	BD*(1)C158-H163	0.14
LP*(3)Al153	BD*(1)C158-H164	0.91
LP(2)O166	BD*(1)C158-H164	0.08
BD*(1)Al153-O166	BD*(1)C158-H163	0.10
BD*(1)Al153-O166	BD*(1)C158-H164	0.16
BD(1)Al153-O166	BD*(1)C168-H170	0.05
LP*(1)Al153	BD*(1)C168-H170	0.21
LP*(2)Al153	BD*(1)C168-H170	1.39
LP*(3)Al153	BD*(1)C168-H170	1.01
LP*(3)Al153	BD*(1)C169-H172	0.11
LP*(3)Al153	BD*(1)C169-H173	2.09
LP*(3)Al153	BD*(1)C169-H174	0.16
LP(1)O166	BD*(1)C168-H170	1.70
LP(2)O166	BD*(1)C168-H170	0.77
BD*(1)Al153-O166	BD*(1)C168-H170	0.42
LP(1)O154	BD*(1)C156-H160	0.71
LP(2)O154	BD*(1)C155-H157	4.32

LP(3)O154	BD*(1)C155-H157	0.58
LP(3)O154	BD*(1)C168-H170	0.06
LP*(2)Al165	BD*(1)C137-H139	0.08
BD(1)Al165-Cl167	BD*(1)C156-H161	0.16
LP*(1)Al165	BD*(1)C156-H161	0.20
LP*(1)Al165	BD*(1)C158-H164	0.11
LP*(2)Al165	BD*(1)C156-H161	0.15
LP*(3)Al165	BD*(1)C156-H160	0.06
LP*(3)Al165	BD*(1)C156-H161	1.00
LP(1)Cl167	BD*(1)C158-H164	0.18
LP(2)Cl167	BD*(1)C156-H161	1.59
LP(2)Cl167	BD*(1)C158-H164	1.23
LP(3)Cl167	BD*(1)C156-H161	0.18
LP(3)Cl167	BD*(1)C158-H164	0.64
BD(1)Al165-Cl167	BD*(1)C171-H175	0.09
LP*(1)Al165	BD*(1)C171-H175	0.08
LP*(2)Al165	BD*(1)C168-H170	0.08
LP*(2)Al165	BD*(1)C171-H175	0.36
LP*(3)Al165	BD*(1)C171-H175	2.22
LP*(3)Al165	BD*(1)C171-H176	0.12
LP(1)Cl167	BD*(1)C169-H174	0.07
LP(2)Cl167	BD*(1)C171-H175	0.23
LP(2)Cl167	BD*(1)C171-H177	0.08
LP(3)Cl167	BD*(1)C168-H170	0.07
LP(3)Cl167	BD*(1)C169-H174	0.65
LP(3)Cl167	BD*(1)C171-H175	0.06
Total		83.4