

Electronic Supplementary Information

Reaction Mechanism of Atomic Layer Deposition of Aluminum Sulfide using Trimethylaluminum and Hydrogen Sulfide

Yanghong Yu, Zhongchao Zhou, Lina Xu^{*}, Yihong Ding, Guoyong Fang^{*}

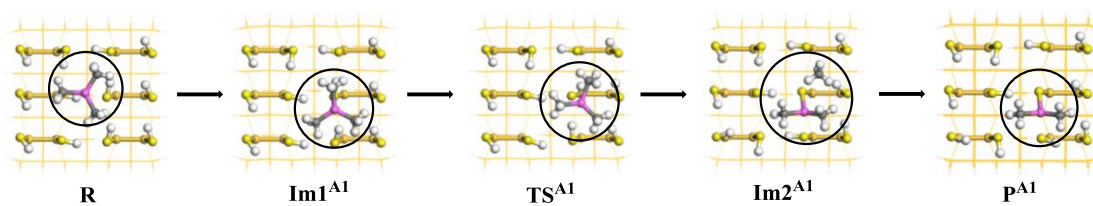
College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou
325035, China. ^{*} Email: xulina@wzu.edu.cn and fanggy@wzu.edu.cn.

Electronic Supplementary Information (ESI) available: Structures of all stationary
points of TMA half-reaction and Cartesian coordinates of all stationary points of
TMA and H₂S half-reactions. See DOI: 10.1039/xxxxxxx

Figure S1. Structures of all stationary points of TMA half-reaction.....S2

Table S1 Atomic coordinates of all stationary points of TMA and H₂S
half-reactions.....S3

(a) A1 section of TMA half reaction



(b) A2 section of TMA half reaction

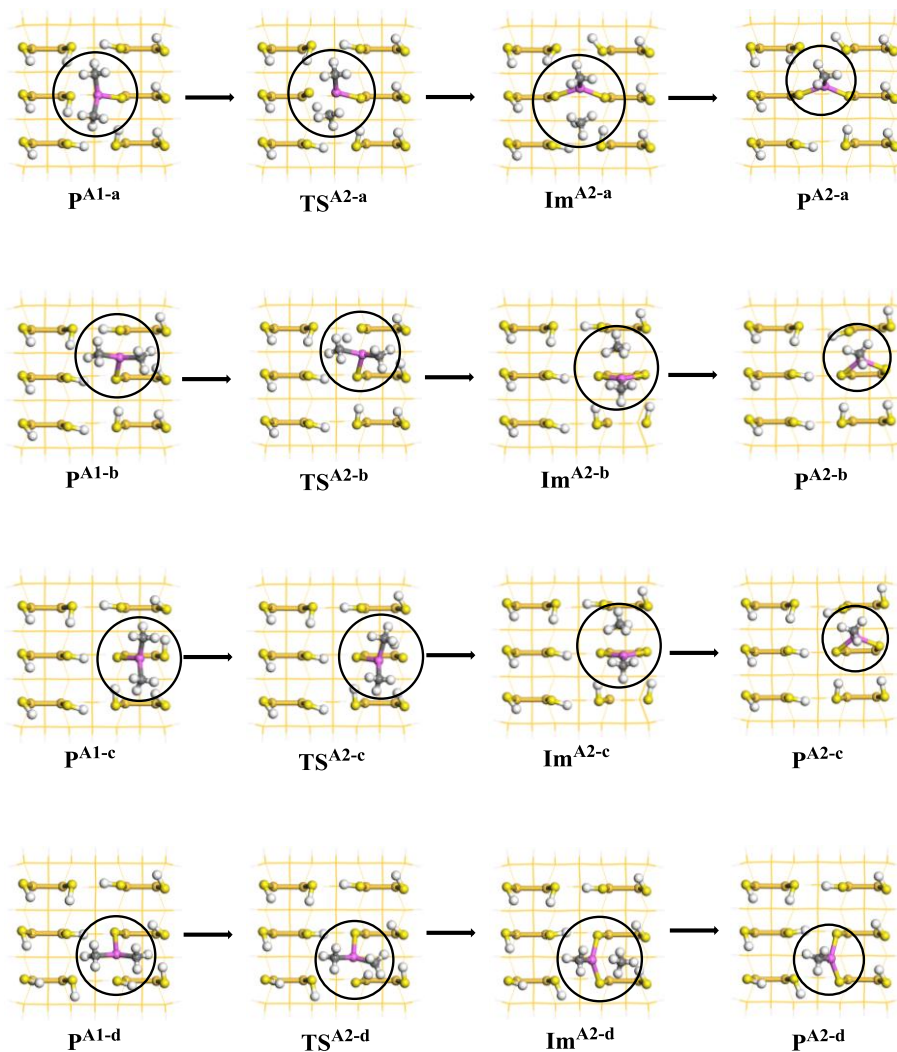


Figure S1. Structures of all stationary points of TMA half-reaction (A1 and A2).

Table S1 Atomic coordinates of all stationary points of TMA and H₂S half-reactions.

Substrate			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000

Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50220000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23580000	1.82410000	-2.71530000
Si	29.31590000	1.82220000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15200000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000

H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03990000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10520000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000

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Si	22.31777800	7.57744100	-0.15272800
Si	22.34152700	11.42553200	-0.11121400
Si	24.80281600	11.41263800	-0.13919300
Si	22.34236400	3.72976600	-0.13346300
Si	24.76865200	7.58066200	-0.14170400
Si	24.79842000	3.73808300	-0.12450400
Si	29.99231200	7.58553900	-0.15802100
Si	29.98910100	11.41814500	-0.13304700
Si	32.43925900	11.42914900	-0.13667600
Si	29.99528000	3.74596100	-0.13685300
Si	32.45180400	7.58515300	-0.14548600
Si	32.45574400	3.73636200	-0.11450700
S	21.62013200	3.90299200	1.90421200
S	25.24840700	3.64867800	1.98622500
S	29.21087900	3.51189000	1.86672200
S	33.20615900	3.53864700	1.89488100
S	21.61545900	11.62397200	1.90758500
S	25.61295700	11.57395500	1.86374700
S	29.54623100	11.42964200	1.99044300
S	33.16981000	11.25136200	1.89912500
S	21.57768500	7.76257600	1.87004700
S	25.18581300	7.61504600	1.98614600
S	29.19001900	7.42587900	1.85337600
S	33.19459700	7.41161000	1.87844300
H	22.37373900	2.89996500	2.39261900

H	26.55862000	3.36830500	1.83968500
H	29.56902200	4.72062900	2.34051500
H	32.78109300	4.73748300	2.33961800
H	22.21275800	10.51882700	2.39327800
H	25.41710800	10.28300000	2.20310700
H	28.21393000	11.60424300	1.85828800
H	32.54031400	12.34375400	2.37062900
H	22.18344500	6.65535100	2.34404600
H	26.51010600	7.38491800	1.86971900
H	29.46935800	8.68575100	2.24838000
H	32.57254100	8.50406200	2.36235100

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Si	21.62780700	9.49439600	-1.35760400
Si	23.54589900	11.41659400	-4.07300800
Si	27.38390000	13.34060700	-2.71530000
Si	25.46399200	13.33852100	-1.35771100
Si	27.38777800	9.50043200	-2.71519000
Si	25.46802400	9.49843500	-1.35779300
Si	27.38600300	11.42049200	-4.07300800
Si	23.55159300	5.65640800	-2.71517700
Si	21.63172800	5.65450300	-1.35777800

Si	23.54980100	7.57649800	-4.07310000
Si	23.55559900	1.81640500	-2.71529600
Si	21.63561400	1.81430600	-1.35768300
Si	23.55369900	3.73639400	-4.07299100
Si	27.39178100	5.66043100	-2.71517600
Si	25.47184000	5.65881800	-1.35757800
Si	27.38989100	7.58039700	-4.07297900
Si	27.39573100	1.82019700	-2.71523600
Si	25.47550700	1.81861700	-1.35779300
Si	27.39380300	3.74030400	-4.07300700
Si	31.22409800	13.34440300	-2.71530400
Si	29.30420200	13.34242400	-1.35780900
Si	31.22787900	9.50429900	-2.71521800
Si	29.30817600	9.50224400	-1.35786500
Si	31.22609900	11.42438900	-4.07301400
Si	33.14420600	13.34619900	-1.35770500
Si	33.14806900	9.50617800	-1.35769600
Si	31.23190500	5.66406800	-2.71518100
Si	29.31190300	5.66220600	-1.35801600
Si	31.22999500	7.58430800	-4.07307300
Si	31.23587100	1.82407700	-2.71533900
Si	29.31584400	1.82211900	-1.35784200
Si	31.23389200	3.74421600	-4.07299000
Si	33.15191900	5.66655200	-1.35742500
Si	33.15564800	1.82637600	-1.35772800
H	23.57340200	14.53380000	-3.62660000

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H	20.30640600	9.52909000	-2.04961200
H	27.38360100	14.60160000	-3.52699900
H	20.37710200	13.01590200	-2.11610400
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H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
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H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21399900	14.54030000	-3.62810100
H	33.24320500	14.57910000	-0.51770000
H	34.41309900	13.07150000	-2.09460200
H	29.29671000	14.53720500	-0.44840700
H	34.47829300	9.54807600	-2.03201500
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47894100	5.68931600	-2.03982000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
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Si	24.80469400	11.41233800	-0.13839900
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S	25.22065800	3.66310900	1.99220600
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S	21.61884000	11.62436200	1.90868500
S	25.62028200	11.57031300	1.86284000
S	29.55132600	11.44000900	1.99456200
S	33.16591200	11.24732200	1.90214400
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S	29.12873700	7.55934800	1.82685600
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H	26.54351400	3.42937200	1.87733700
H	29.55868400	4.73533900	2.32406600
H	32.57203500	4.64588600	2.40497300
H	22.21582600	10.51877000	2.39384700
H	25.42136900	10.28015400	2.20405000
H	28.21996500	11.63074700	1.87137800
H	32.53065500	12.33528300	2.37605100
H	22.18384100	6.65643200	2.34471500
H	26.49536000	7.38702800	1.88788200
H	29.33108100	8.86003100	2.13452300
H	32.56536200	8.51214100	2.35425600
Al	29.22142600	6.63956900	4.50194100
C	27.59580800	5.53635400	4.34388800
C	29.05966500	8.54533800	4.97033300

C	30.96322200	5.73794000	4.64668300
H	27.78759600	4.48539900	4.58607900
H	26.80245400	5.88709000	5.01195500
H	27.16896000	5.55328600	3.33567500
H	28.17487100	9.01024000	4.52139400
H	28.95849600	8.67308000	6.05381800
H	29.93408000	9.12963000	4.66513000
H	30.95042600	4.69931500	4.30132300
H	31.75684700	6.26855000	4.11335500
H	31.26680500	5.70775900	5.70024300
TS ^{A1}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000

Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50220000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31190000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000

H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
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H	28.55730000	11.37890000	-4.97570000
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H	24.40090000	7.58990000	-5.29000000
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H	33.24320000	14.57910000	-0.51770000
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H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000

H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
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H	23.57410000	0.63100000	-3.64310000
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H	22.14230000	3.73350000	-4.61450000
Si	22.31560200	7.57773500	-0.15341600
Si	22.34173900	11.42550800	-0.11140700
Si	24.80285200	11.41224100	-0.13843900
Si	22.34385000	3.73080600	-0.13287000
Si	24.76725400	7.57980500	-0.13665500
Si	24.79963800	3.73707400	-0.12409100
Si	30.00770000	7.58768400	-0.14345200
Si	29.97886700	11.42288300	-0.13460400
Si	32.43003200	11.43212500	-0.13710100
Si	29.98375000	3.74514200	-0.14233700
Si	32.46724600	7.58275300	-0.13959100
Si	32.44631700	3.73477400	-0.11606300
S	21.63166300	3.90740800	1.90780600
S	25.26931200	3.62381700	1.98410200
S	29.16447700	3.59279100	1.85965800

S	33.17959900	3.53763300	1.89853900
S	21.61550700	11.62460200	1.90724000
S	25.60945800	11.56440900	1.86632600
S	29.52263500	11.50542400	1.97373800
S	33.14816500	11.28867400	1.91260300
S	21.56396300	7.76425400	1.86489400
S	25.15418900	7.59864500	1.99738700
S	29.06342300	7.53516700	1.81586800
S	33.23781500	7.41144300	1.87191100
H	22.39676700	2.91292400	2.39622900
H	26.54081600	3.21314500	1.81024000
H	29.09674500	4.92158700	2.06997800
H	32.56974700	4.63105400	2.39395800
H	22.21298200	10.51980700	2.39356400
H	25.43263900	10.26714700	2.19272200
H	28.19102600	11.66967600	1.82824700
H	32.38389000	12.28519600	2.39790200
H	22.16704500	6.65758000	2.34331900
H	26.48126200	7.37369100	1.90711000
H	29.86386400	8.41726000	2.83312100
H	32.89207800	8.65280700	2.26477800
Al	29.83294200	7.02012800	4.18576200
C	27.98969500	6.90164100	4.82889300
C	30.51598000	8.97086100	4.19231200
C	31.19096900	5.66442000	4.52828400
H	27.94103100	6.81166800	5.91861200

H	27.40180200	7.78072300	4.54779100
H	27.48174400	6.02421500	4.41382800
H	29.75063800	9.67987900	4.51250500
H	31.14800900	8.74103300	5.06629300
H	31.18577700	9.49371600	3.50499300
H	30.96033800	4.69892400	4.06959400
H	32.19214200	5.96984100	4.21807800
H	31.22439300	5.48983300	5.61035200
Im2 ^{A1}			
Si	-3.93336800	5.77348800	-1.83893300
Si	-5.85336800	5.77158800	-0.48133300
Si	-3.92956800	1.93338800	-1.83883300
Si	-5.84956800	1.93128800	-0.48123300
Si	-3.93146800	3.85348800	-3.19663300
Si	-0.09346800	5.77748800	-1.83893300
Si	-2.01336800	5.77538800	-0.48133300
Si	-0.08956800	1.93728800	-1.83883300
Si	-2.00936800	1.93528800	-0.48143300
Si	-0.09136800	3.85738800	-3.19663300
Si	-3.92576800	-1.90671200	-1.83883300
Si	-5.84566800	-1.90861200	-0.48143300
Si	-3.92756800	0.01338800	-3.19673300
Si	-3.92176800	-5.74671200	-1.83893300
Si	-5.84176800	-5.74881200	-0.48133300
Si	-3.92366800	-3.82671200	-3.19663300

Si	-0.08556800	-1.90271200	-1.83883300
Si	-2.00556800	-1.90431200	-0.48123300
Si	-0.08746800	0.01728800	-3.19663300
Si	-0.08166800	-5.74291200	-1.83883300
Si	-2.00186800	-5.74451200	-0.48143300
Si	-0.08356800	-3.82281200	-3.19663300
Si	3.74673200	5.78128800	-1.83893300
Si	1.82683200	5.77928800	-0.48143300
Si	3.75053200	1.94118800	-1.83883300
Si	1.83083200	1.93908800	-0.48153300
Si	3.74873200	3.86128800	-3.19663300
Si	5.66683200	5.78308800	-0.48133300
Si	5.67073200	1.94308800	-0.48133300
Si	3.75453200	-1.89901200	-1.83883300
Si	1.83453200	-1.90091200	-0.48163300
Si	3.75263200	0.02118800	-3.19673300
Si	3.75853200	-5.73901200	-1.83893300
Si	1.83843200	-5.74101200	-0.48143300
Si	3.75653200	-3.81891200	-3.19663300
Si	5.67453200	-1.89651200	-0.48103300
Si	5.67823200	-5.73671200	-0.48133300
H	-3.90396800	6.97068800	-2.75023300
H	-1.99606800	6.96298800	0.43976700
H	-7.17096800	1.96598800	-1.17323300
H	-0.09376800	7.03848800	-2.65063300
H	-7.10026800	5.45278800	-1.23973300

H	-5.98266800	7.02858800	0.31336700
H	-3.06876800	3.88118800	-4.40173300
H	-5.34356800	3.86598800	-3.73433300
H	1.07993200	3.81578800	-4.09933300
H	-1.26466800	3.80778800	-4.09593300
H	-3.07646800	0.02678800	-4.41363300
H	-5.34226800	0.02328800	-3.73443300
H	1.07763200	0.03278800	-4.10963300
H	-1.27516800	0.03108800	-4.07903300
H	1.08333200	-3.76361200	-4.10503300
H	-1.25876800	-3.75911200	-4.09303300
H	3.73663200	6.97718800	-2.75173300
H	5.76583200	7.01598800	0.35866700
H	6.93573200	5.50838800	-1.21823300
H	1.81933200	6.97408800	0.42796700
H	7.00093200	1.98498800	-1.15563300
H	5.16203200	3.86768800	-3.73233300
H	2.88643200	3.88838800	-4.40133300
H	7.00153200	-1.87381200	-1.16343300
H	5.16243200	0.03498800	-3.74583300
H	2.88653200	0.03738800	-4.40133300
H	1.83293200	-6.94161200	0.41726700
H	3.75123200	-6.92611200	-2.76383300
H	6.93803200	-5.44441200	-1.22873300
H	5.78803200	-6.97881200	0.33876700
H	5.16923200	-3.80871200	-3.73443300

H	2.89363200	-3.82771200	-4.40143300
H	-0.07766800	-6.99331200	-2.66703300
H	-5.94996800	-6.99381200	0.33436700
H	-7.09786800	-5.46001200	-1.23633300
H	-7.16516800	-1.87931200	-1.17833300
H	-3.90326800	-6.93211200	-2.76673300
H	-1.98266800	-6.94191200	0.42186700
H	-3.06146800	-3.83981200	-4.40263300
H	-5.33506800	-3.82961200	-3.73813300
Si	-5.16628400	0.01338300	0.72398700
Si	-5.13448700	3.86145800	0.76391300
Si	-2.67499600	3.84875200	0.74102300
Si	-5.13732700	-3.83534500	0.75812900
Si	-2.70947600	0.01487400	0.73795500
Si	-2.67962800	-3.82077200	0.71841000
Si	2.48902000	0.01226400	0.77404400
Si	2.50494000	3.86195300	0.75264900
Si	4.95671100	3.86413100	0.74679200
Si	2.54369100	-3.80297100	0.70025500
Si	4.95837400	0.02558600	0.72416400
Si	4.99665100	-3.82485900	0.76253500
S	-5.73831800	-3.88134200	2.84541200
S	-1.93297200	-3.80069100	2.76817300
S	1.90474900	-3.85838000	2.82644600
S	5.67873800	-4.00406500	2.79692700
S	-5.86031900	4.04303400	2.78554900

S	-1.87524700	3.99086400	2.74647600
S	2.07754500	3.97402700	2.86280300
S	5.66913900	3.68652800	2.78649500
S	-5.95915900	0.18713000	2.72749500
S	-2.24062700	-0.03729300	2.85340100
S	1.71124100	0.09049300	2.75134300
S	5.71826100	-0.06640900	2.74636900
H	-4.52503900	-3.53990400	3.32751200
H	-2.04453700	-5.13024300	2.95470500
H	0.57377300	-3.79444400	2.58194400
H	5.49560800	-2.71165200	3.13307900
H	-5.24622900	2.94669000	3.27045200
H	-2.05789100	2.69492200	3.07258000
H	0.74522800	4.13051400	2.73134200
H	5.05171800	4.79675500	3.23311200
H	-5.62712200	-1.05461500	3.13019900
H	-0.89414200	-0.06612700	2.69679200
H	3.24857700	1.97068500	4.69116800
H	4.75213400	0.71278500	3.27593700
Al	2.02173100	-1.71474400	4.14970600
C	0.32178900	-1.91311000	5.10469100
C	3.38098500	1.54787100	5.68701200
C	3.67098600	-1.97413900	5.17342000
H	0.31031400	-2.81916400	5.72004400
H	0.19183700	-1.06665500	5.78918800
H	-0.55900900	-1.93792200	4.45941800

H	2.48497400	0.98420200	5.95360900
H	4.24438100	0.88180100	5.70623000
H	3.52907300	2.35131500	6.40819300
H	3.88282400	-3.04274700	5.28407900
H	4.57039700	-1.48872500	4.79702900
H	3.48911200	-1.58104800	6.17989500
P ^{Al}			
Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200

Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000

H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700

H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31249200	7.57639300	-0.13990000
Si	22.32575500	11.42533100	-0.11265300
Si	24.77908600	11.41527000	-0.14019200
Si	22.33260700	3.72899500	-0.13555800
Si	24.77460700	7.57610800	-0.18493700
Si	24.78350700	3.74038300	-0.13836900
Si	29.97161800	7.58248900	-0.09746600
Si	29.99005900	11.42392400	-0.13367100
Si	32.43944400	11.42627700	-0.13687600
Si	29.97898800	3.74736000	-0.14184400
Si	32.44787900	7.58264700	-0.14984100
Si	32.44359800	3.73723700	-0.11412300
S	21.62127800	3.91150400	1.90677400
S	25.21893800	3.72196300	1.98627100
S	29.15672000	3.57825900	1.85317200
S	33.15783700	3.54800400	1.90737700
S	21.58461800	11.61746700	1.90135700
S	25.55130700	11.63024000	1.86759700
S	29.55694300	11.51444200	1.97894000

S	33.16028400	11.24890500	1.89851200
S	21.58305600	7.76676600	1.88401500
S	25.46406600	7.61896700	1.92091600
S	29.65105500	7.45589600	2.00487400
S	33.24546700	7.42042400	1.85019000
H	22.34675500	2.88670900	2.39186200
H	26.55114000	3.53042600	1.86220900
H	29.38945800	4.86173700	2.20637300
H	32.57116600	4.66846400	2.37240900
H	22.17303300	10.50817300	2.38766100
H	25.18216300	10.42462600	2.34194600
H	28.25725600	11.83748800	1.83532700
H	32.52873200	12.34511300	2.35893500
H	22.17814900	6.65531700	2.35910900
H	25.23712500	6.31251300	2.19403900
H	32.45637200	8.37304000	2.38501800
Al	27.72283800	7.72647400	3.17876500
C	27.35490100	6.05496800	4.13524100
C	27.47512400	9.44414700	4.06409500
H	26.43844700	6.11417800	4.73130900
H	27.26281200	5.19298200	3.47092600
H	28.17451000	5.83667000	4.82853000
H	28.31438500	9.61411000	4.74687800
H	27.44234300	10.29933200	3.39231800
H	26.55889700	9.43824400	4.66394900

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Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
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Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300

Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000

H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000

H	22.14230000	3.73350000	-4.61450000
Si	22.31249200	7.57639300	-0.13990000
Si	22.32575500	11.42533100	-0.11265300
Si	24.77908600	11.41527000	-0.14019200
Si	22.33260700	3.72899500	-0.13555800
Si	24.77460700	7.57610800	-0.18493700
Si	24.78350700	3.74038300	-0.13836900
Si	29.97161800	7.58248900	-0.09746600
Si	29.99005900	11.42392400	-0.13367100
Si	32.43944400	11.42627700	-0.13687600
Si	29.97898800	3.74736000	-0.14184400
Si	32.44787900	7.58264700	-0.14984100
Si	32.44359800	3.73723700	-0.11412300
S	21.62127800	3.91150400	1.90677400
S	25.21893800	3.72196300	1.98627100
S	29.15672000	3.57825900	1.85317200
S	33.15783700	3.54800400	1.90737700
S	21.58461800	11.61746700	1.90135700
S	25.55130700	11.63024000	1.86759700
S	29.55694300	11.51444200	1.97894000
S	33.16028400	11.24890500	1.89851200
S	21.58305600	7.76676600	1.88401500
S	25.46406600	7.61896700	1.92091600
S	29.65105500	7.45589600	2.00487400
S	33.24546700	7.42042400	1.85019000
H	22.34675500	2.88670900	2.39186200

H	26.55114000	3.53042600	1.86220900
H	29.38945800	4.86173700	2.20637300
H	32.57116600	4.66846400	2.37240900
H	22.17303300	10.50817300	2.38766100
H	25.18216300	10.42462600	2.34194600
H	28.25725600	11.83748800	1.83532700
H	32.52873200	12.34511300	2.35893500
H	22.17814900	6.65531700	2.35910900
H	25.23712500	6.31251300	2.19403900
H	32.45637200	8.37304000	2.38501800
Al	27.72283800	7.72647400	3.17876500
C	27.35490100	6.05496800	4.13524100
C	27.47512400	9.44414700	4.06409500
H	26.43844700	6.11417800	4.73130900
H	27.26281200	5.19298200	3.47092600
H	28.17451000	5.83667000	4.82853000
H	28.31438500	9.61411000	4.74687800
H	27.44234300	10.29933200	3.39231800
H	26.55889700	9.43824400	4.66394900
TS ^{A2-a}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000

Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50200000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000

Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000

H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32580100	7.57517800	-0.14068000
Si	22.33105500	11.42444600	-0.11168400
Si	24.78815200	11.42037300	-0.13652900
Si	22.33250700	3.72948000	-0.13615500
Si	24.79301000	7.57902600	-0.16106300
Si	24.78368400	3.74087900	-0.13805600

Si	29.96818700	7.58188600	-0.11623100
Si	29.98279000	11.41990700	-0.13146900
Si	32.43494000	11.42724000	-0.13269700
Si	29.98795000	3.74530800	-0.14357100
Si	32.44342700	7.58198100	-0.14625100
Si	32.44997300	3.73701700	-0.11638600
S	21.61560800	3.90065000	1.90405900
S	25.22319500	3.71367900	1.97835900
S	29.20085600	3.54451700	1.86257700
S	33.17775200	3.54859700	1.90138500
S	21.59381300	11.60657600	1.90501600
S	25.56063800	11.72585800	1.86079900
S	29.51097400	11.45864900	1.97907500
S	33.13578200	11.25805300	1.91213000
S	21.59661400	7.75539700	1.88362700
S	25.36989500	7.89802000	1.93095400
S	29.56211600	7.44620000	1.98593400
S	33.20428200	7.41616200	1.86847200
H	22.34847600	2.87847300	2.38383600
H	26.53669800	3.43396100	1.84324000
H	29.48849500	4.80727000	2.24523600
H	32.59521500	4.66867200	2.37168900
H	22.18269300	10.49235600	2.38034100
H	25.20302700	10.53505300	2.37448600
H	28.21603400	11.79901400	1.82432900
H	32.39604900	12.27924700	2.38392000

H	22.23050800	6.66538100	2.35899400
H	26.03101100	6.74965300	2.73191400
H	32.44602000	8.40891600	2.37405400
Al	27.58258500	7.92342600	2.92669500
C	27.06215000	6.12025200	3.79576700
C	27.49244700	9.39336200	4.19773900
H	26.15279100	5.91708900	4.36845400
H	27.34335500	5.22208400	3.24941800
H	27.83991100	6.28724300	4.55938900
H	28.41416400	9.43030700	4.78658600
H	27.37501400	10.36973500	3.72639100
H	26.65599800	9.24815300	4.88850500
Im1 ^{A2-a}			
Si	-3.84644600	5.74337700	-1.76963200
Si	-5.76644600	5.74147700	-0.41203200
Si	-3.84264600	1.90327700	-1.76953200
Si	-5.76264600	1.90117700	-0.41193200
Si	-3.84454600	3.82337700	-3.12733200
Si	-0.00654600	5.74737700	-1.76963200
Si	-1.92644600	5.74527700	-0.41203200
Si	-0.00274600	1.90717700	-1.76953200
Si	-1.92254600	1.90527700	-0.41213200
Si	-0.00444600	3.82727700	-3.12733200
Si	-3.83884600	-1.93682300	-1.76953200
Si	-5.75874600	-1.93872300	-0.41213200

Si	-3.84064600	-0.01672300	-3.12743200
Si	-3.83484600	-5.77682300	-1.76963200
Si	-5.75484600	-5.77892300	-0.41203200
Si	-3.83674600	-3.85682300	-3.12733200
Si	0.00135400	-1.93282300	-1.76953200
Si	-1.91864600	-1.93432300	-0.41193200
Si	-0.00054600	-0.01282300	-3.12733200
Si	0.00525400	-5.77302300	-1.76953200
Si	-1.91494600	-5.77462300	-0.41213200
Si	0.00335400	-3.85292300	-3.12733200
Si	3.83365400	5.75117700	-1.76963200
Si	1.91375400	5.74917700	-0.41213200
Si	3.83745400	1.91107700	-1.76953200
Si	1.91775400	1.90877700	-0.41223200
Si	3.83565400	3.83117700	-3.12733200
Si	5.75375400	5.75297700	-0.41203200
Si	5.75765400	1.91297700	-0.41203200
Si	3.84145400	-1.92912300	-1.76953200
Si	1.92155400	-1.93102300	-0.41233200
Si	3.83955400	-0.00892300	-3.12743200
Si	3.84545400	-5.76912300	-1.76963200
Si	1.92535400	-5.77112300	-0.41213200
Si	3.84345400	-3.84902300	-3.12733200
Si	5.76145400	-1.92662300	-0.41173200
Si	5.76515400	-5.76682300	-0.41203200
H	-3.81704600	6.94057700	-2.68093200

H	-1.90914600	6.93287700	0.50906800
H	-7.08404600	1.93587700	-1.10393200
H	-0.00684600	7.00837700	-2.58133200
H	-7.01334600	5.42267700	-1.17043200
H	-5.89574600	6.99847700	0.38266800
H	-2.98184600	3.85107700	-4.33243200
H	-5.25664600	3.83587700	-3.66503200
H	1.16685400	3.78567700	-4.03003200
H	-1.17774600	3.77767700	-4.02663200
H	-2.98954600	-0.00332300	-4.34433200
H	-5.25534600	-0.00682300	-3.66513200
H	1.16455400	0.00267700	-4.04033200
H	-1.18824600	0.00097700	-4.00973200
H	1.17025400	-3.79372300	-4.03573200
H	-1.17184600	-3.78922300	-4.02373200
H	3.82355400	6.94707700	-2.68243200
H	5.85275400	6.98587700	0.42796800
H	7.02265400	5.47827700	-1.14893200
H	1.90625400	6.94397700	0.49726800
H	7.08785400	1.95487700	-1.08633200
H	5.24895400	3.83757700	-3.66303200
H	2.97335400	3.85827700	-4.33203200
H	7.08845400	-1.90392300	-1.09413200
H	5.24935400	0.00487700	-3.67653200
H	2.97345400	0.00727700	-4.33203200
H	1.91985400	-6.97172300	0.48656800

H	3.83815400	-6.95622300	-2.69453200
H	7.02495400	-5.47452300	-1.15943200
H	5.87495400	-7.00892300	0.40806800
H	5.25615400	-3.83882300	-3.66513200
H	2.98055400	-3.85782300	-4.33213200
H	0.00925400	-7.02342300	-2.59773200
H	-5.86304600	-7.02392300	0.40366800
H	-7.01094600	-5.49012300	-1.16703200
H	-7.07824600	-1.90942300	-1.10903200
H	-3.81634600	-6.96222300	-2.69743200
H	-1.89574600	-6.97202300	0.49116800
H	-2.97454600	-3.86992300	-4.33333200
H	-5.24814600	-3.85972300	-3.66883200
Si	-5.03133700	-0.01944500	0.80644900
Si	-5.06759800	3.83108300	0.83036900
Si	-2.60794200	3.81862600	0.81174400
Si	-5.05167100	-3.86342000	0.81189900
Si	-2.54877400	-0.00608400	0.81279900
Si	-2.59583100	-3.85191800	0.81923400
Si	2.57596300	-0.00522200	0.80159600
Si	2.57998000	3.81792600	0.80713100
Si	5.03784100	3.83201000	0.82151700
Si	2.59388800	-3.84290700	0.80984900
Si	5.04751100	-0.01311800	0.80154500
Si	5.05675600	-3.85795400	0.83161000
S	-5.77485000	-3.69055800	2.84861900

S	-2.16795700	-3.89326700	2.93620000
S	1.78854700	-3.96582900	2.81777000
S	5.78590500	-4.06012100	2.84784700
S	-5.82938500	4.01239800	2.83868800
S	-1.88797800	3.99889300	2.84818000
S	1.87116000	3.77307800	2.87484500
S	5.69419300	3.64992200	2.87818700
S	-5.75892800	0.13682600	2.83869700
S	-1.97566500	0.12373500	2.88811400
S	2.05424800	0.00859200	2.89627800
S	5.75153500	-0.19391200	2.83518400
H	-5.05106400	-4.72044400	3.32573200
H	-0.83974400	-4.09796300	2.81382600
H	1.95947400	-2.66302300	3.12625600
H	5.19039000	-2.95392900	3.33343300
H	-5.48504000	2.77506200	3.24669200
H	-2.61807100	2.98069600	3.34388100
H	1.03925700	4.82113500	2.75321200
H	4.88349800	4.61550100	3.35158900
H	-4.98576400	-0.84815700	3.33712700
H	-0.30630000	-2.03009700	4.38237700
H	4.99770900	0.81137600	3.32234400
Al	0.05680300	0.78433900	3.49564400
C	0.09299300	-2.01708500	5.39874300
C	0.04069500	1.61894800	5.24423000
H	-0.64357400	-1.57170100	6.06725500

H	0.28902900	-3.04375100	5.70933600
H	1.02482300	-1.45015500	5.44258200
H	1.02422400	1.54731800	5.71468500
H	-0.21791900	2.67793000	5.16605500
H	-0.69685100	1.14100800	5.89408300
P ^{A2-a}			
Si	-3.84640000	5.74340000	-1.76960000
Si	-5.76640000	5.74150000	-0.41200000
Si	-3.84260000	1.90330000	-1.76950000
Si	-5.76260000	1.90120000	-0.41190000
Si	-3.84450000	3.82340000	-3.12730000
Si	-0.00650000	5.74740000	-1.76960000
Si	-1.92640000	5.74530000	-0.41200000
Si	-0.00270000	1.90720000	-1.76950000
Si	-1.92250000	1.90530000	-0.41210000
Si	-0.00440000	3.82730000	-3.12730000
Si	-3.83880000	-1.93680000	-1.76950000
Si	-5.75870000	-1.93870000	-0.41210000
Si	-3.84060000	-0.01670000	-3.12740000
Si	-3.83480000	-5.77680000	-1.76960000
Si	-5.75480000	-5.77890000	-0.41200000
Si	-3.83670000	-3.85680000	-3.12730000
Si	0.00140000	-1.93280000	-1.76950000
Si	-1.91860000	-1.93430000	-0.41190000
Si	-0.00050000	-0.01280000	-3.12730000

Si	0.00530000	-5.77300000	-1.76950000
Si	-1.91490000	-5.77460000	-0.41210000
Si	0.00340000	-3.85290000	-3.12730000
Si	3.83370000	5.75120000	-1.76960000
Si	1.91380000	5.74920000	-0.41210000
Si	3.83750000	1.91110000	-1.76950000
Si	1.91780000	1.90880000	-0.41220000
Si	3.83570000	3.83120000	-3.12730000
Si	5.75380000	5.75300000	-0.41200000
Si	5.75770000	1.91300000	-0.41200000
Si	3.84150000	-1.92910000	-1.76950000
Si	1.92160000	-1.93100000	-0.41230000
Si	3.83960000	-0.00890000	-3.12740000
Si	3.84550000	-5.76910000	-1.76960000
Si	1.92540000	-5.77110000	-0.41210000
Si	3.84350000	-3.84900000	-3.12730000
Si	5.76150000	-1.92660000	-0.41170000
Si	5.76520000	-5.76680000	-0.41200000
H	-3.81700000	6.94060000	-2.68090000
H	-1.90910000	6.93290000	0.50910000
H	-7.08400000	1.93590000	-1.10390000
H	-0.00680000	7.00840000	-2.58130000
H	-7.01330000	5.42270000	-1.17040000
H	-5.89570000	6.99850000	0.38270000
H	-2.98180000	3.85110000	-4.33240000
H	-5.25660000	3.83590000	-3.66500000

H	1.16690000	3.78570000	-4.03000000
H	-1.17770000	3.77770000	-4.02660000
H	-2.98950000	-0.00330000	-4.34430000
H	-5.25530000	-0.00680000	-3.66510000
H	1.16460000	0.00270000	-4.04030000
H	-1.18820000	0.00100000	-4.00970000
H	1.17030000	-3.79370000	-4.03570000
H	-1.17180000	-3.78920000	-4.02370000
H	3.82360000	6.94710000	-2.68240000
H	5.85280000	6.98590000	0.42800000
H	7.02270000	5.47830000	-1.14890000
H	1.90630000	6.94400000	0.49730000
H	7.08790000	1.95490000	-1.08630000
H	5.24900000	3.83760000	-3.66300000
H	2.97340000	3.85830000	-4.33200000
H	7.08850000	-1.90390000	-1.09410000
H	5.24940000	0.00490000	-3.67650000
H	2.97350000	0.00730000	-4.33200000
H	1.91990000	-6.97170000	0.48660000
H	3.83820000	-6.95620000	-2.69450000
H	7.02500000	-5.47450000	-1.15940000
H	5.87500000	-7.00890000	0.40810000
H	5.25620000	-3.83880000	-3.66510000
H	2.98060000	-3.85780000	-4.33210000
H	0.00930000	-7.02340000	-2.59770000
H	-5.86300000	-7.02390000	0.40370000

H	-7.01090000	-5.49010000	-1.16700000
H	-7.07820000	-1.90940000	-1.10900000
H	-3.81630000	-6.96220000	-2.69740000
H	-1.89570000	-6.97200000	0.49120000
H	-2.97450000	-3.86990000	-4.33330000
H	-5.24810000	-3.85970000	-3.66880000
Si	-5.02732600	-0.01934400	0.80835300
Si	-5.06979700	3.83105200	0.82960100
Si	-2.61129200	3.81947300	0.80863600
Si	-5.05129100	-3.86364400	0.81163600
Si	-2.54165500	-0.00476900	0.81734100
Si	-2.59521300	-3.85158100	0.82070400
Si	2.57587000	-0.00559800	0.80609400
Si	2.57841800	3.81671400	0.80392300
Si	5.03713500	3.83214000	0.82315500
Si	2.59436000	-3.84377200	0.80850400
Si	5.04773300	-0.01343400	0.80178500
Si	5.05707400	-3.85810000	0.83121300
S	-5.77765500	-3.69062600	2.84717500
S	-2.16608300	-3.88775900	2.93588900
S	1.79050800	-3.97326100	2.81508100
S	5.78899000	-4.06171800	2.84616700
S	-5.83124300	4.01335400	2.83779700
S	-1.89676700	4.00739600	2.84581000
S	1.84434400	3.75077300	2.86528900
S	5.68798500	3.65001800	2.88152600

S	-5.75597500	0.13834700	2.84025800
S	-1.94215900	0.14335700	2.88607900
S	2.05241600	0.01759800	2.90277300
S	5.75439700	-0.19508500	2.83426100
H	-5.05350200	-4.71970900	3.32541900
H	-0.83582800	-4.07023500	2.80804300
H	1.95161500	-2.66857300	3.11783600
H	5.19558900	-2.95538000	3.33382000
H	-5.49188800	2.77449300	3.24539800
H	-2.62621800	2.98941700	3.34265100
H	1.02449400	4.80913400	2.75349300
H	4.87550700	4.61508500	3.35298300
H	-4.98370700	-0.84677400	3.33971200
H	4.99725600	0.80635100	3.32418500
Al	0.07709700	0.87584000	3.46261400
C	0.05906200	1.69679500	5.21785500
H	1.07587500	1.83949800	5.58939000
H	-0.43267300	2.67213200	5.18997900
H	-0.48899000	1.07036600	5.92723700
P^{A1-b}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000

Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50220000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31190000	5.66220000	-1.35800000

Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000

H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31905400	7.57751100	-0.15278900
Si	22.34005800	11.42551500	-0.11074600
Si	24.80118800	11.41169600	-0.14514900
Si	22.34350900	3.72989700	-0.13308200
Si	24.76980700	7.57730800	-0.14131700
Si	24.79963700	3.73784000	-0.12306600

Si	29.96812500	7.59151500	-0.11207000
Si	30.01399100	11.40403000	-0.17211600
Si	32.46286600	11.43022700	-0.13482700
Si	29.98273300	3.74814500	-0.13340500
Si	32.43758900	7.58150300	-0.14268000
Si	32.44607800	3.73588900	-0.11431000
S	21.62002900	3.90653600	1.90391100
S	25.25015800	3.64709500	1.98599300
S	29.19005400	3.58619300	1.87233300
S	33.18490000	3.54009600	1.89885400
S	21.62367500	11.62670700	1.91067200
S	25.62029800	11.56022500	1.85928500
S	29.44755500	11.44053200	1.97865200
S	33.18659900	11.32924700	1.90219200
S	21.58081600	7.76745900	1.87008400
S	25.18574300	7.59524600	1.98274300
S	29.13487400	7.48900300	1.85030100
S	33.18260300	7.41719000	1.87921700
H	22.37612800	2.90668000	2.39501900
H	26.56220600	3.37276600	1.83656600
H	29.33686300	4.88837500	2.19573000
H	32.59182700	4.64788800	2.38367000
H	22.21798100	10.51854300	2.39340300
H	25.41715600	10.26815700	2.19007600
H	28.10469700	11.53548900	1.80044500
H	32.69125900	12.52714800	2.26523800

H	22.18954200	6.66268500	2.34620600
H	26.50540900	7.32478100	1.86882800
H	32.39930700	8.38615800	2.38823100
Al	29.40222000	9.28216700	3.27485600
C	27.69668500	9.57069100	4.19556000
C	31.04971800	9.31742200	4.33093700
H	27.56272200	10.61191100	4.50788300
H	26.82547600	9.28310600	3.60474800
H	27.67519400	8.96565500	5.10862000
H	31.35616800	8.30198300	4.60286400
H	31.90799600	9.82004800	3.88385300
H	30.82641200	9.84389500	5.26551200
TS ^{A2-b}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000

Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50220000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31190000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000

H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000

H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32047300	7.57762600	-0.15316600
Si	22.33878300	11.42521300	-0.11470000
Si	24.79876900	11.41587500	-0.14116000
Si	22.34300100	3.72980800	-0.13342200
Si	24.77061800	7.57909400	-0.14543300
Si	24.79889000	3.73757200	-0.12391200
Si	29.99383900	7.59286500	-0.13441700
Si	29.98655400	11.40336200	-0.14021700
Si	32.44997900	11.42956700	-0.14111800
Si	29.98365600	3.74842000	-0.13554400
Si	32.45565300	7.58334900	-0.14579100
Si	32.44537400	3.73652900	-0.11532800
S	21.62087500	3.90271200	1.90466700

S	25.25014000	3.63776800	1.98576300
S	29.19212900	3.58557800	1.87195500
S	33.17481900	3.54600200	1.90330000
S	21.60064100	11.61546400	1.90162500
S	25.59316600	11.59587800	1.85794900
S	29.57570200	11.47070100	2.01440700
S	33.23329400	11.27704400	1.87701100
S	21.58962400	7.76118600	1.87403300
S	25.19895000	7.58357700	1.97902900
S	29.21128000	7.51186100	1.85933700
S	33.23116700	7.39783600	1.86473500
H	22.37594800	2.90061600	2.39277700
H	26.55868800	3.35035900	1.83415300
H	29.35319300	4.88324900	2.20344900
H	32.56780300	4.64526600	2.39032800
H	22.18730800	10.50266200	2.38248700
H	25.16631200	10.38165500	2.26089200
H	28.38499700	10.68684800	2.65216500
H	32.50551500	12.28808400	2.38575400
H	22.19741900	6.65318900	2.34378000
H	26.51938700	7.32668100	1.85082700
H	32.80123300	8.59685300	2.30434600
Al	29.67880200	9.34151800	3.11382200
C	27.78807600	9.76028000	3.82720200
C	31.07531200	9.24520900	4.46577500
H	27.53820600	10.66636600	4.38453800

H	26.92637300	9.43164300	3.24945700
H	27.94361000	8.98201500	4.59409300
H	31.32921400	8.20553800	4.69174300
H	31.99215400	9.75815600	4.16752900
H	30.72915000	9.71423600	5.39202600
Im1 ^{A2-b}			
Si	-3.90810000	5.70174600	-1.77306200
Si	-5.82810000	5.69984600	-0.41546200
Si	-3.90430000	1.86164600	-1.77296200
Si	-5.82430000	1.85954600	-0.41536200
Si	-3.90620000	3.78174600	-3.13076200
Si	-0.06820000	5.70574600	-1.77306200
Si	-1.98810000	5.70364600	-0.41546200
Si	-0.06430000	1.86554600	-1.77296200
Si	-1.98410000	1.86354600	-0.41556200
Si	-0.06610000	3.78564600	-3.13076200
Si	-3.90050000	-1.97845400	-1.77296200
Si	-5.82040000	-1.98035400	-0.41556200
Si	-3.90230000	-0.05835400	-3.13086200
Si	-3.89650000	-5.81845400	-1.77306200
Si	-5.81650000	-5.82055400	-0.41546200
Si	-3.89840000	-3.89845400	-3.13076200
Si	-0.06030000	-1.97445400	-1.77296200
Si	-1.98030000	-1.97605400	-0.41536200
Si	-0.06220000	-0.05445400	-3.13076200

Si	-0.05640000	-5.81465400	-1.77296200
Si	-1.97660000	-5.81625400	-0.41556200
Si	-0.05830000	-3.89455400	-3.13076200
Si	3.77200000	5.70954600	-1.77306200
Si	1.85210000	5.70754600	-0.41556200
Si	3.77580000	1.86944600	-1.77296200
Si	1.85610000	1.86734600	-0.41566200
Si	3.77400000	3.78954600	-3.13076200
Si	5.69210000	5.71134600	-0.41546200
Si	5.69600000	1.87134600	-0.41546200
Si	3.77980000	-1.97075400	-1.77296200
Si	1.85980000	-1.97265400	-0.41576200
Si	3.77790000	-0.05055400	-3.13086200
Si	3.78380000	-5.81075400	-1.77306200
Si	1.86370000	-5.81275400	-0.41556200
Si	3.78180000	-3.89065400	-3.13076200
Si	5.69980000	-1.96825400	-0.41516200
Si	5.70350000	-5.80845400	-0.41546200
H	-3.87870000	6.89894600	-2.68436200
H	-1.97080000	6.89124600	0.50563800
H	-7.14570000	1.89424600	-1.10736200
H	-0.06850000	6.96674600	-2.58476200
H	-7.07500000	5.38104600	-1.17386200
H	-5.95740000	6.95684600	0.37923800
H	-3.04350000	3.80944600	-4.33586200
H	-5.31830000	3.79424600	-3.66846200

H	1.10520000	3.74404600	-4.03346200
H	-1.23940000	3.73604600	-4.03006200
H	-3.05120000	-0.04495400	-4.34776200
H	-5.31700000	-0.04845400	-3.66856200
H	1.10290000	-0.03895400	-4.04376200
H	-1.24990000	-0.04065400	-4.01316200
H	1.10860000	-3.83535400	-4.03916200
H	-1.23350000	-3.83085400	-4.02716200
H	3.76190000	6.90544600	-2.68586200
H	5.79110000	6.94424600	0.42453800
H	6.96100000	5.43664600	-1.15236200
H	1.84460000	6.90234600	0.49383800
H	7.02620000	1.91324600	-1.08976200
H	5.18730000	3.79594600	-3.66646200
H	2.91170000	3.81664600	-4.33546200
H	7.02680000	-1.94555400	-1.09756200
H	5.18770000	-0.03675400	-3.67996200
H	2.91180000	-0.03435400	-4.33546200
H	1.85820000	-7.01335400	0.48313800
H	3.77650000	-6.99785400	-2.69796200
H	6.96330000	-5.51615400	-1.16286200
H	5.81330000	-7.05055400	0.40463800
H	5.19450000	-3.88045400	-3.66856200
H	2.91890000	-3.89945400	-4.33556200
H	-0.05240000	-7.06505400	-2.60116200
H	-5.92470000	-7.06555400	0.40023800

H	-7.07260000	-5.53175400	-1.17046200
H	-7.13990000	-1.95105400	-1.11246200
H	-3.87800000	-7.00385400	-2.70086200
H	-1.95740000	-7.01365400	0.48773800
H	-3.03620000	-3.91155400	-4.33676200
H	-5.30980000	-3.90135400	-3.67226200
Si	-5.12810600	-0.05735400	0.79122100
Si	-5.11280200	3.79042300	0.82569100
Si	-2.65308000	3.77934600	0.81168000
Si	-5.10995800	-3.90526700	0.80815700
Si	-2.67617800	-0.05464200	0.79723400
Si	-2.65404400	-3.89719400	0.81752100
Si	2.55310100	-0.03496500	0.79434200
Si	2.50427500	3.77591900	0.80991800
Si	4.95894100	3.78828800	0.79842000
Si	2.53418400	-3.88522600	0.80544100
Si	5.01464700	-0.05334400	0.78816500
Si	4.99456000	-3.89937300	0.82757400
S	-5.83261200	-3.73596000	2.84645300
S	-2.20608200	-3.99800700	2.92840700
S	1.74331600	-4.02947600	2.81665900
S	5.71835800	-4.10443800	2.84682400
S	-5.86331600	3.97901500	2.83790100
S	-1.88764000	3.92683700	2.82025300
S	1.84369800	3.86650400	2.85713700
S	5.58242600	3.55831900	2.87633100

S	-5.85182400	0.12183500	2.82187200
S	-2.22856300	-0.03496000	2.92055200
S	1.86551600	-0.04114400	2.84699300
S	5.82521400	-0.27978700	2.78357300
H	-5.08044100	-4.74135000	3.33217400
H	-0.89644900	-4.28053600	2.77954500
H	1.91879500	-2.73413300	3.14716000
H	5.11026100	-3.00936800	3.34133900
H	-5.26928500	2.87274200	3.32453000
H	-2.29510000	2.69260000	3.18091500
H	-0.28240000	2.04677300	4.33457800
H	4.78471300	4.52630300	3.36742600
H	-5.24305100	-0.98761900	3.28686200
H	-0.89778600	-0.21870400	2.78641600
H	5.46806800	0.92954700	3.25309500
Al	2.36475600	1.92543500	3.77298000
C	-0.32748600	1.68013400	5.36416700
C	3.10642400	1.88286900	5.56085900
H	0.23654400	2.33609600	6.02786600
H	-1.37561600	1.67836900	5.66382200
H	0.05877600	0.66122300	5.42519500
H	2.67995800	1.06668700	6.14863800
H	4.18838500	1.72677800	5.52053200
H	2.92701400	2.82405200	6.08625600
p ^{A2-b}			

Si	-3.90810000	5.70170100	-1.77310000
Si	-5.82809800	5.69979800	-0.41550300
Si	-3.90430000	1.86159900	-1.77300000
Si	-5.82429500	1.85949600	-0.41540200
Si	-3.90620000	3.78170000	-3.13080000
Si	-0.06818200	5.70569300	-1.77313800
Si	-1.98809400	5.70359600	-0.41549800
Si	-0.06442400	1.86549000	-1.77282400
Si	-1.98410000	1.86350700	-0.41559400
Si	-0.06609700	3.78558500	-3.13080300
Si	-3.90050000	-1.97850300	-1.77300000
Si	-5.82039800	-1.98039900	-0.41560000
Si	-3.90230000	-0.05840000	-3.13090100
Si	-3.89650000	-5.81850000	-1.77310000
Si	-5.81650100	-5.82060000	-0.41550000
Si	-3.89840000	-3.89850000	-3.13079900
Si	-0.06024600	-1.97448900	-1.77308000
Si	-1.98030200	-1.97609700	-0.41540200
Si	-0.06220000	-0.05448500	-3.13080300
Si	-0.05639200	-5.81470500	-1.77301100
Si	-1.97660100	-5.81630600	-0.41560100
Si	-0.05830000	-3.89460000	-3.13079400
Si	3.77200900	5.70954400	-1.77309500
Si	1.85236200	5.70736900	-0.41539900
Si	3.77576600	1.86941800	-1.77297400
Si	1.85591100	1.86732100	-0.41623300

Si	3.77400600	3.78950100	-3.13075600
Si	5.69207900	5.71131000	-0.41527600
Si	5.69608400	1.87130800	-0.41591500
Si	3.77982000	-1.97086200	-1.77298900
Si	1.85990400	-1.97253900	-0.41553100
Si	3.77790100	-0.05062100	-3.13086800
Si	3.78380000	-5.81080400	-1.77311300
Si	1.86365400	-5.81282400	-0.41559900
Si	3.78179800	-3.89067900	-3.13083400
Si	5.69975300	-1.96829000	-0.41497800
Si	5.70349400	-5.80850000	-0.41552100
H	-3.87870000	6.89890000	-2.68439900
H	-1.97080400	6.89120200	0.50559800
H	-7.14570100	1.89420100	-1.10739800
H	-0.06849800	6.96670300	-2.58479700
H	-7.07500100	5.38100100	-1.17389900
H	-5.95740000	6.95680000	0.37920000
H	-3.04350000	3.80940000	-4.33590000
H	-5.31830000	3.79420000	-3.66850000
H	1.10520000	3.74400000	-4.03350000
H	-1.23940000	3.73600000	-4.03010000
H	-3.05120000	-0.04500000	-4.34780000
H	-5.31700000	-0.04850000	-3.66860000
H	1.10290000	-0.03900000	-4.04380000
H	-1.24990000	-0.04070000	-4.01320000
H	1.10860000	-3.83540000	-4.03920000

H	-1.23350000	-3.83090000	-4.02720000
H	3.76189900	6.90536700	-2.68594300
H	5.79111200	6.94422200	0.42446600
H	6.96096400	5.43657200	-1.15245000
H	1.84446200	6.90230200	0.49379600
H	7.02625900	1.91319900	-1.08968400
H	5.18730000	3.79590000	-3.66650000
H	2.91170000	3.81660000	-4.33550000
H	7.02677700	-1.94558600	-1.09764300
H	5.18770000	-0.03680000	-3.68000000
H	2.91180000	-0.03440000	-4.33550000
H	1.85822000	-7.01340700	0.48309100
H	3.77650000	-6.99790400	-2.69799500
H	6.96329700	-5.51620200	-1.16290700
H	5.81330300	-7.05060000	0.40459900
H	5.19450000	-3.88050000	-3.66860000
H	2.91890000	-3.89950000	-4.33560000
H	-0.05240000	-7.06510000	-2.60120000
H	-5.92470100	-7.06560000	0.40020000
H	-7.07260000	-5.53180000	-1.17050000
H	-7.13990000	-1.95110000	-1.11249900
H	-3.87800000	-7.00390000	-2.70090000
H	-1.95740100	-7.01370000	0.48769900
H	-3.03620000	-3.91160000	-4.33680000
H	-5.30980000	-3.90140000	-3.67230000
Si	-5.13294400	-0.05554100	0.78725800

Si	-5.11173900	3.79131300	0.83299700
Si	-2.64536100	3.76743800	0.81143000
Si	-5.10872800	-3.90448500	0.81024900
Si	-2.68356700	-0.06267500	0.79601100
Si	-2.65304400	-3.89802400	0.81769900
Si	2.51998400	-0.02892800	0.79637400
Si	2.52549600	3.78038600	0.80653800
Si	4.98230600	3.79154500	0.81219300
Si	2.53731900	-3.88456800	0.80533600
Si	4.99002100	-0.05116800	0.80355500
Si	4.99902100	-3.89983900	0.82639400
S	-5.82280200	-3.72528000	2.85006200
S	-2.18684000	-4.00614700	2.92595100
S	1.74723600	-4.01757500	2.81881800
S	5.73338600	-4.11017800	2.84032000
S	-5.85758500	3.99303100	2.84597000
S	-1.83972000	3.76463500	2.83237300
S	1.86417000	3.94794200	2.85227600
S	5.64403200	3.62706900	2.87289000
S	-5.85401800	0.13906800	2.81683900
S	-2.27361600	-0.13642500	2.92919100
S	1.68019900	-0.00095200	2.79764900
S	5.71183700	-0.25583500	2.82879300
H	-5.06568400	-4.72584300	3.33840300
H	-0.89100300	-4.33780100	2.76259700
H	1.89815600	-2.71544100	3.13356200

H	5.14097300	-3.00717300	3.33604700
H	-5.28921000	2.87406500	3.33352500
H	-2.48842100	2.64709600	3.21533800
H	4.65940100	4.39995400	3.36980500
H	-5.23679200	-0.96194400	3.29073300
H	-1.03414500	-0.65688800	2.83239500
H	5.11294600	0.85516500	3.29952900
Al	1.10061800	2.01180200	3.54713400
C	0.17060400	1.96254000	5.24345100
H	-0.73967500	1.36094700	5.18232500
H	0.80482400	1.51888500	6.01613300
H	-0.10494200	2.96992700	5.56320500
P^{Al-c}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49649900	-2.71520000
Si	21.62780200	9.49440000	-1.35759900
Si	23.54590000	11.41660000	-4.07300100
Si	27.38389800	13.34060400	-2.71529800
Si	25.46399800	13.33850100	-1.35770300
Si	27.38783000	9.50041700	-2.71523600
Si	25.46800000	9.49839800	-1.35780000
Si	27.38600300	11.42049400	-4.07300600
Si	23.55160000	5.65640100	-2.71520000
Si	21.63170100	5.65450000	-1.35779900

Si	23.54980000	7.57650000	-4.07309900
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180200	5.66037400	-2.71520200
Si	25.47180100	5.65880100	-1.35759800
Si	27.38990100	7.58040100	-4.07300300
Si	27.39570200	1.82019700	-2.71520200
Si	25.47549800	1.81860000	-1.35780300
Si	27.39380000	3.74030300	-4.07300000
Si	31.22409400	13.34440800	-2.71529500
Si	29.30418900	13.34244400	-1.35779500
Si	31.22791800	9.50439200	-2.71516500
Si	29.30812300	9.50237800	-1.35788200
Si	31.22609900	11.42441900	-4.07297000
Si	33.14419300	13.34624200	-1.35769100
Si	33.14819300	9.50637300	-1.35769200
Si	31.23189500	5.66402000	-2.71518700
Si	29.31179900	5.66201700	-1.35798900
Si	31.23000600	7.58429900	-4.07313700
Si	31.23589800	1.82409400	-2.71529900
Si	29.31579500	1.82205200	-1.35779300
Si	31.23389700	3.74418300	-4.07297200
Si	33.15198500	5.66643600	-1.35738700
Si	33.15560600	1.82635800	-1.35769300
H	23.57340000	14.53380000	-3.62660000

H	25.48129900	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360200	14.60159900	-3.52700200
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21399900	14.54029800	-3.62810200
H	33.24320300	14.57910100	-0.51770200
H	34.41309500	13.07150100	-2.09460800
H	29.29670700	14.53720500	-0.44840600
H	34.47828300	9.54813000	-2.03203100
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47888100	5.68926500	-2.03983700
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030400	0.62149600	-0.45910500

H	31.22860000	0.63700300	-3.64020400
H	34.41540100	2.11869700	-2.10509900
H	33.26539600	0.58429700	-0.53760500
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970200	0.56980200	-3.54340300
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32578600	7.57743000	-0.14994900
Si	22.34342000	11.42577300	-0.11117500
Si	24.80567000	11.41294600	-0.13764600
Si	22.34158600	3.73025900	-0.13438500
Si	24.78012900	7.57969300	-0.13929300
Si	24.79707200	3.73650000	-0.12338000
Si	29.95076800	7.57903200	-0.10708500
Si	29.97458000	11.42139200	-0.12153000
Si	32.43184100	11.43850900	-0.13869900
Si	29.96732900	3.74559100	-0.14115700
Si	32.40080000	7.58108300	-0.18634000
Si	32.43173900	3.73605200	-0.11824400
S	21.61912600	3.90463800	1.90296100

S	25.24357800	3.62141300	1.98699800
S	29.14172200	3.60162200	1.85158700
S	33.14860500	3.59740000	1.91221100
S	21.61775600	11.62516300	1.90771000
S	25.62262800	11.57596200	1.86096900
S	29.55627600	11.48902000	1.99142600
S	33.23876400	11.32873400	1.88443400
S	21.59539900	7.76369000	1.87643600
S	25.23430300	7.61003000	1.98136400
S	29.28173200	7.48078400	1.91048900
S	33.06549700	7.54393600	1.94404600
H	22.37422100	2.90277400	2.39156400
H	26.53461200	3.26797300	1.83091100
H	29.08612700	4.93530000	2.06484700
H	32.34753300	4.55383300	2.41839700
H	22.21720000	10.52163300	2.39446300
H	25.45480800	10.27949100	2.19423100
H	28.22262000	11.66073200	1.88241900
H	32.29235700	12.07942300	2.47923000
H	22.20535200	6.65779300	2.34823800
H	26.56259100	7.39878200	1.85505300
H	33.12155500	8.88850600	2.10468500
Al	31.03226200	7.44097900	3.42048800
C	31.28145800	9.10713100	4.40724800
C	31.14254300	5.74445100	4.39583000
H	32.21574000	9.09789600	4.97864400

H	31.28168900	9.98734000	3.76332100
H	30.46761200	9.23992300	5.12762300
H	30.52238800	5.84624600	5.29433500
H	30.79892400	4.84293500	3.88551800
H	32.16294500	5.56245200	4.75096700
TS ^{A2-c}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000

Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50440000	-2.71520000
Si	29.30810000	9.50240000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14820000	9.50640000	-1.35770000
Si	31.23190000	5.66400000	-2.71520000
Si	29.31180000	5.66200000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15200000	5.66640000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000

H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000

H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32210500	7.57765300	-0.15131100
Si	22.34428800	11.42582500	-0.11071800
Si	24.80680300	11.41216500	-0.13751300
Si	22.34243000	3.73046600	-0.13387900
Si	24.77480600	7.57912400	-0.14165100
Si	24.79770900	3.73635100	-0.12414900
Si	29.96330700	7.58081200	-0.13499800
Si	29.99265400	11.42092300	-0.12106300
Si	32.44679400	11.43753700	-0.14534400
Si	29.97629800	3.74529100	-0.13850600
Si	32.41376300	7.58863800	-0.15701700
Si	32.44197100	3.73297500	-0.11421300
S	21.62505000	3.90532200	1.90540200
S	25.25606200	3.61649900	1.98481500
S	29.15168500	3.58346000	1.85868200
S	33.18817800	3.50462000	1.89729800
S	21.61863500	11.62485700	1.90857800
S	25.62987000	11.55892200	1.86039700
S	29.60667900	11.47662200	2.00198100
S	33.27838100	11.35547500	1.85642600

S	21.58934200	7.76379700	1.87435200
S	25.21407300	7.59745400	1.98381700
S	29.24608800	7.47968200	1.88540700
S	33.04186000	7.45115100	1.94044800
H	22.38442800	2.90612400	2.39298000
H	26.53578900	3.22837400	1.81810800
H	29.05327700	4.91233500	2.07052100
H	32.59604600	4.59494500	2.41759700
H	22.21809600	10.52119200	2.39490300
H	25.44029600	10.26435300	2.18936800
H	28.26083600	11.52088700	1.91170600
H	32.67707900	12.47877100	2.29224800
H	22.19612800	6.65609700	2.34589600
H	26.53730100	7.35886100	1.86511300
H	32.32475900	8.55423700	2.82267900
Al	31.02850200	7.24912800	3.24606300
C	31.49808800	9.04266100	4.10225300
C	31.03013300	5.76509100	4.50248500
H	32.12971200	8.85705700	4.97471100
H	31.79942600	9.99013200	3.65021900
H	30.46867500	9.23156800	4.44009000
H	30.25107300	5.91437300	5.25729400
H	30.84380000	4.79345200	4.03842200
H	31.98550200	5.70620600	5.03257700
Im1 ^{A2-c}			

Si	-3.95506500	5.76397200	-1.77896600
Si	-5.87506500	5.76207200	-0.42136600
Si	-3.95126500	1.92387200	-1.77886600
Si	-5.87126500	1.92177200	-0.42126600
Si	-3.95316500	3.84397200	-3.13666600
Si	-0.11516500	5.76797200	-1.77896600
Si	-2.03506500	5.76587200	-0.42136600
Si	-0.11126500	1.92777200	-1.77886600
Si	-2.03106500	1.92577200	-0.42146600
Si	-0.11306500	3.84787200	-3.13666600
Si	-3.94746500	-1.91622800	-1.77886600
Si	-5.86736500	-1.91812800	-0.42146600
Si	-3.94926500	0.00387200	-3.13676600
Si	-3.94346500	-5.75622800	-1.77896600
Si	-5.86346500	-5.75832800	-0.42136600
Si	-3.94536500	-3.83622800	-3.13666600
Si	-0.10726500	-1.91222800	-1.77886600
Si	-2.02726500	-1.91382800	-0.42126600
Si	-0.10916500	0.00777200	-3.13666600
Si	-0.10336500	-5.75242800	-1.77886600
Si	-2.02356500	-5.75402800	-0.42146600
Si	-0.10526500	-3.83232800	-3.13666600
Si	3.72503500	5.77177200	-1.77896600
Si	1.80513500	5.76977200	-0.42146600
Si	3.72883500	1.93177200	-1.77886600
Si	1.80903500	1.92977200	-0.42156600

Si	3.72703500	3.85177200	-3.13666600
Si	5.64513500	5.77357200	-0.42136600
Si	5.64913500	1.93377200	-0.42136600
Si	3.73283500	-1.90862800	-1.77886600
Si	1.81273500	-1.91062800	-0.42166600
Si	3.73093500	0.01167200	-3.13676600
Si	3.73683500	-5.74852800	-1.77896600
Si	1.81673500	-5.75052800	-0.42146600
Si	3.73483500	-3.82842800	-3.13666600
Si	5.65293500	-1.90622800	-0.42106600
Si	5.65653500	-5.74622800	-0.42136600
H	-3.92566500	6.96117200	-2.69026600
H	-2.01776500	6.95347200	0.49973400
H	-7.19266500	1.95647200	-1.11326600
H	-0.11546500	7.02897200	-2.59066600
H	-7.12196500	5.44327200	-1.17976600
H	-6.00436500	7.01907200	0.37333400
H	-3.09046500	3.87167200	-4.34176600
H	-5.36526500	3.85647200	-3.67436600
H	1.05823500	3.80627200	-4.03936600
H	-1.28636500	3.79827200	-4.03596600
H	-3.09816500	0.01727200	-4.35366600
H	-5.36396500	0.01377200	-3.67446600
H	1.05593500	0.02327200	-4.04966600
H	-1.29686500	0.02157200	-4.01906600
H	1.06163500	-3.77312800	-4.04506600

H	-1.28046500	-3.76862800	-4.03306600
H	3.71493500	6.96767200	-2.69176600
H	5.74413500	7.00647200	0.41863400
H	6.91403500	5.49887200	-1.15826600
H	1.79763500	6.96457200	0.48793400
H	6.97923500	1.97547200	-1.09566600
H	5.14033500	3.85817200	-3.67236600
H	2.86473500	3.87887200	-4.34136600
H	6.97983500	-1.88332800	-1.10346600
H	5.14073500	0.02547200	-3.68586600
H	2.86483500	0.02787200	-4.34136600
H	1.81123500	-6.95112800	0.47723400
H	3.72953500	-6.93562800	-2.70386600
H	6.91633500	-5.45392800	-1.16876600
H	5.76633500	-6.98832800	0.39873400
H	5.14753500	-3.81822800	-3.67446600
H	2.87193500	-3.83722800	-4.34146600
H	-0.09936500	-7.00282800	-2.60706600
H	-5.97166500	-7.00332800	0.39433400
H	-7.11956500	-5.46952800	-1.17636600
H	-7.18686500	-1.88882800	-1.11836600
H	-3.92496500	-6.94162800	-2.70676600
H	-2.00436500	-6.95142800	0.48183400
H	-3.08316500	-3.84932800	-4.34266600
H	-5.35676500	-3.83912800	-3.67816600
Si	-5.17622100	0.00534800	0.78533100

Si	-5.15696600	3.85323800	0.82473100
Si	-2.69573700	3.83972900	0.79899000
Si	-5.15653000	-3.84219600	0.80274600
Si	-2.72411200	0.00617300	0.79235800
Si	-2.70140600	-3.83600300	0.81131600
Si	2.49183400	0.01024900	0.78259400
Si	2.49148900	3.84994000	0.81156300
Si	4.94436600	3.85863400	0.80680200
Si	2.48749200	-3.82848600	0.79894000
Si	4.94788600	0.01673200	0.79088300
Si	4.95716900	-3.83289900	0.82349000
S	-5.87137800	-3.66725900	2.84290400
S	-2.23661800	-3.95183600	2.91947400
S	1.66541200	-4.02250000	2.79844100
S	5.71063900	-3.89747300	2.85660400
S	-5.88661300	4.05281800	2.84258500
S	-1.88688300	3.98777800	2.80247300
S	2.06345700	3.90789800	2.92612200
S	5.68882100	3.76263000	2.84215700
S	-5.90143400	0.19200400	2.81368700
S	-2.27219300	0.01603600	2.91734700
S	1.82177900	-0.07943500	2.84141500
S	5.58769200	0.03255400	2.85802700
H	-5.11152000	-4.66658900	3.32951100
H	-0.95743900	-4.33965800	2.74781300
H	1.57851500	-2.70309200	3.05501200

H	5.99103700	-2.58411100	2.94718600
H	-5.28763500	2.94993100	3.33107100
H	-2.06820200	2.69139500	3.12829100
H	0.72141400	3.96987200	2.79558700
H	5.26346100	4.99895400	3.16664900
H	-5.29333300	-0.91595500	3.28300800
H	-0.96032400	-0.26943900	2.78966400
H	4.08137400	2.19629400	4.72708800
Al	3.71096300	-0.32898100	3.95401400
C	3.46449200	2.20733100	5.63166500
C	3.71649500	-1.16009200	5.69734800
H	3.96164300	1.68187100	6.44643400
H	3.32404600	3.25444700	5.89856800
H	2.48141100	1.77278400	5.44044000
H	2.83401500	-0.88989800	6.28127200
H	3.71690300	-2.24769900	5.57111600
H	4.60726400	-0.89304800	6.27031900
P^{A2-c}			
Si	-3.95510900	5.76400800	-1.77899700
Si	-5.87509900	5.76209600	-0.42139900
Si	-3.95130400	1.92387400	-1.77889600
Si	-5.87130900	1.92180200	-0.42131400
Si	-3.95319900	3.84400000	-3.13670500
Si	-0.11530400	5.76807900	-1.77885400
Si	-2.03512600	5.76581200	-0.42148400

Si	-0.11248700	1.92848600	-1.77675100
Si	-2.03113400	1.92572800	-0.42157600
Si	-0.11293600	3.84765800	-3.13707100
Si	-3.94750400	-1.91616100	-1.77889700
Si	-5.86740700	-1.91809900	-0.42151500
Si	-3.94931100	0.00390100	-3.13677600
Si	-3.94351000	-5.75620900	-1.77899900
Si	-5.86349900	-5.75829600	-0.42140400
Si	-3.94539800	-3.83620000	-3.13670700
Si	-0.10878900	-1.91301800	-1.77638500
Si	-2.02731800	-1.91368200	-0.42135600
Si	-0.10884800	0.00778900	-3.13734300
Si	-0.10356200	-5.75251900	-1.77868400
Si	-2.02362100	-5.75390000	-0.42158300
Si	-0.10513900	-3.83206700	-3.13706000
Si	3.72498500	5.77196400	-1.77878000
Si	1.80544500	5.76993600	-0.42174200
Si	3.72882000	1.93027600	-1.78094000
Si	1.81117300	1.92839500	-0.42226500
Si	3.72697900	3.85236400	-3.13584200
Si	5.64483800	5.77389500	-0.42174600
Si	5.64628700	1.93127000	-0.42374200
Si	3.73277100	-1.90701600	-1.78161300
Si	1.81746200	-1.90895200	-0.42242700
Si	3.73088600	0.01173100	-3.13627100
Si	3.73678500	-5.74858100	-1.77882200

Si	1.81704300	-5.75065100	-0.42184300
Si	3.73477700	-3.82901800	-3.13580700
Si	5.64798700	-1.90405000	-0.42359400
Si	5.65621400	-5.74644400	-0.42179200
H	-3.92570400	6.96120700	-2.69029200
H	-2.01778900	6.95349800	0.49970200
H	-7.19271200	1.95649600	-1.11327800
H	-0.11547500	7.02898000	-2.59073100
H	-7.12200600	5.44330100	-1.17979000
H	-6.00439000	7.01910100	0.37330000
H	-3.09050000	3.87170000	-4.34180000
H	-5.36530000	3.85650000	-3.67440000
H	1.05820000	3.80630000	-4.03940000
H	-1.28640000	3.79830000	-4.03600000
H	-3.09820000	0.01730000	-4.35370000
H	-5.36400000	0.01380000	-3.67450000
H	1.05590000	0.02330000	-4.04970000
H	-1.29690000	0.02160000	-4.01910000
H	1.06160000	-3.77310000	-4.04510000
H	-1.28050000	-3.76860000	-4.03310000
H	3.71489200	6.96767100	-2.69183800
H	5.74420400	7.00648100	0.41861500
H	6.91405100	5.49894500	-1.15822900
H	1.79751200	6.96457200	0.48793600
H	6.98055000	1.97656700	-1.09292000
H	5.14030000	3.85820000	-3.67240000

H	2.86470000	3.87890000	-4.34140000
H	6.98141400	-1.88422400	-1.10032500
H	5.14070000	0.02550000	-3.68590000
H	2.86480000	0.02790000	-4.34140000
H	1.81113800	-6.95106300	0.47724900
H	3.72949500	-6.93558800	-2.70391500
H	6.91640900	-5.45397700	-1.16864600
H	5.76634500	-6.98827800	0.39872800
H	5.14750000	-3.81820000	-3.67450000
H	2.87190000	-3.83720000	-4.34150000
H	-0.09936900	-7.00278000	-2.60713000
H	-5.97168900	-7.00330100	0.39430000
H	-7.11960700	-5.46950200	-1.17638900
H	-7.18691200	-1.88879700	-1.11837700
H	-3.92500500	-6.94160800	-2.70679000
H	-2.00439300	-6.95139900	0.48180100
H	-3.08320000	-3.84930000	-4.34270000
H	-5.35680000	-3.83910000	-3.67820000
Si	-5.17956200	0.00446100	0.78406600
Si	-5.14790700	3.85337800	0.82953700
Si	-2.67988500	3.83677600	0.79809800
Si	-5.15598000	-3.84295200	0.80290200
Si	-2.72750600	0.00719200	0.79659500
Si	-2.70002900	-3.83466200	0.81243100
Si	2.44470100	-0.00011800	0.77214300
Si	2.56108500	3.81232000	0.77697400

Si	4.99958100	3.86064100	0.79551100
Si	2.49253700	-3.82562000	0.80184800
Si	4.89443300	0.04445500	0.82015900
Si	4.95603200	-3.82588600	0.81798700
S	-5.87988300	-3.66851100	2.84022800
S	-2.24936500	-3.92418000	2.92181600
S	1.69462000	-4.02410900	2.80143300
S	5.72278500	-3.84820700	2.83491000
S	-5.86571700	4.05151000	2.85208200
S	-1.79098200	3.96411100	2.77052700
S	2.30473800	3.50313500	2.96723800
S	5.73490500	3.88638500	2.84200700
S	-5.91991500	0.19102200	2.80710900
S	-2.31056700	0.04048000	2.92530300
S	1.69553000	-0.07985600	2.78488900
S	5.30048600	0.38503600	2.90746500
H	-5.12408000	-4.66904000	3.33041800
H	-0.93570700	-4.19095400	2.77200500
H	1.88992600	-2.74166600	3.16916600
H	5.47973000	-2.54439800	3.08383200
H	-5.27279000	2.94126400	3.33161600
H	-2.12582200	2.71213000	3.14729500
H	0.99932800	3.15623100	2.93367300
H	5.54238400	5.21056300	2.99297100
H	-5.31500900	-0.91672400	3.28113600
H	-0.98224900	-0.17175100	2.81779700

Al	3.32696100	1.16421300	3.70595900
C	3.31817800	1.58934900	5.59586800
H	2.33147300	1.91319300	5.93627300
H	3.61275400	0.72141700	6.19177300
H	4.02688800	2.39466100	5.80719900
p^{Al-d}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180200	5.66039900	-2.71520300
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000

Si	27.39569800	1.82019900	-2.71519700
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30819500	9.50219700	-1.35790200
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190200	5.66410300	-2.71519700
Si	29.31191100	5.66220700	-1.35798900
Si	31.23000000	7.58430000	-4.07310000
Si	31.23589800	1.82410200	-2.71530300
Si	29.31578900	1.82211200	-1.35781400
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660500	-1.35739200
Si	33.15560000	1.82640500	-1.35770800
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000

H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030300	0.62149900	-0.45910100
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000

H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.30891000	7.57729900	-0.15268100
Si	22.34279900	11.42502200	-0.11198800
Si	24.80284500	11.41153300	-0.13574000
Si	22.35723900	3.72908700	-0.11654500
Si	24.76199900	7.57727700	-0.14133800
Si	24.82444400	3.74390000	-0.15022100
Si	29.95227700	7.57704700	-0.10225000
Si	29.98410000	11.42399800	-0.11920800
Si	32.43679400	11.42827900	-0.13139600
Si	30.00986300	3.75746000	-0.16612000
Si	32.42627400	7.58860900	-0.14512400
Si	32.47551900	3.73731700	-0.12313500
S	21.75838500	3.81836500	1.97102600
S	25.66361000	3.75961500	1.85498700
S	29.33195200	3.69606500	1.95520600
S	33.18124900	3.53823000	1.90959000
S	21.61762400	11.61671800	1.90844800
S	25.60614400	11.55217800	1.86846900
S	29.56866600	11.51909800	1.99341100
S	33.17749400	11.25722700	1.89781600

S	21.53090300	7.76883400	1.85266900
S	25.19271200	7.52872200	1.97952200
S	29.12049400	7.67845900	1.85328600
S	33.17312000	7.48749400	1.88443400
H	22.97958100	3.51681100	2.45589000
H	25.87089500	2.43089400	1.92096400
H	30.54470500	3.32627800	2.43016300
H	33.03406400	4.83378700	2.25055500
H	22.22562600	10.51806200	2.39576600
H	25.41560600	10.25755100	2.19563500
H	28.23564000	11.67448000	1.86664700
H	32.56128500	12.36532900	2.35093000
H	21.93387700	6.55545500	2.28082300
H	26.53943400	7.49119100	1.84162100
H	32.20513300	8.26698100	2.40983600
Al	29.29329400	5.87380400	3.25925100
C	27.60575800	5.73419600	4.23486800
C	30.95102700	5.65346300	4.27789400
H	27.49945600	6.60369000	4.89389800
H	26.71336200	5.68873600	3.60999400
H	27.60240000	4.84753700	4.87785200
H	31.02458800	4.65006800	4.71227100
H	31.87246800	5.85519500	3.73418600
H	30.92219700	6.35457400	5.11984700
TS ^{A2-d}			

Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38780000	9.50040000	-2.71520000
Si	25.46800000	9.49840000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65880000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50220000	-1.35790000

Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31190000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000

H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.30614900	7.57666300	-0.15227700

Si	22.34169100	11.42476200	-0.11210500
Si	24.80140600	11.41234500	-0.13672000
Si	22.34837700	3.72937700	-0.11982200
Si	24.75878500	7.57867500	-0.14575000
Si	24.81357200	3.74550000	-0.14215200
Si	29.95896300	7.57031800	-0.11900100
Si	29.98533300	11.42254400	-0.12142400
Si	32.43791300	11.42927100	-0.13174500
Si	30.00564700	3.75580600	-0.14382200
Si	32.43043100	7.58853100	-0.14818300
Si	32.47201200	3.73797400	-0.11924600
S	21.72539100	3.81999800	1.96003500
S	25.57652500	3.78659900	1.89299300
S	29.21746900	3.59157200	1.88902100
S	33.26887400	3.57353900	1.87926000
S	21.61658600	11.61463300	1.90873500
S	25.60287400	11.56953600	1.86721700
S	29.56508700	11.49332300	1.99270700
S	33.17611300	11.27561800	1.90058600
S	21.52703800	7.76929500	1.85263900
S	25.19458300	7.56694800	1.97823600
S	29.16159700	7.64061300	1.87257000
S	33.16448100	7.52499500	1.89203700
H	22.94062500	3.51299400	2.45695900
H	25.84549900	2.46985300	1.96187600
H	30.28813500	4.24999700	2.84197000

H	33.12406400	4.87181600	2.20640300
H	22.22282600	10.51421300	2.39432300
H	25.38233400	10.28565500	2.21590800
H	28.23218600	11.65092300	1.86551500
H	32.56067700	12.38897800	2.34151000
H	21.90527200	6.54640500	2.27587600
H	26.54015600	7.57950600	1.83553500
H	32.19760500	8.32510200	2.38715500
Al	29.05839700	5.69896100	3.01754800
C	27.58259600	5.66690500	4.28344300
C	30.85819600	5.25211800	3.94502200
H	27.71056100	6.46048900	5.02721200
H	26.60550300	5.80123200	3.81656300
H	27.56197900	4.71406900	4.82184600
H	31.34927400	4.30048700	4.17508000
H	31.62105100	5.93226800	3.56598800
H	30.51013800	5.62020300	4.91988900
Im1 ^{A2-d}			
Si	-3.90130800	5.81338800	-1.77140700
Si	-5.82130800	5.81148800	-0.41380700
Si	-3.89750900	1.97328800	-1.77130700
Si	-5.81750800	1.97118800	-0.41370700
Si	-3.89940800	3.89338800	-3.12910700
Si	-0.06140500	5.81739100	-1.77141200
Si	-1.98131000	5.81528900	-0.41381000

Si	-0.05747700	1.97719700	-1.77133900
Si	-1.97731100	1.97518800	-0.41391200
Si	-0.05930200	3.89727900	-3.12911700
Si	-3.89370800	-1.86681000	-1.77130600
Si	-5.81360600	-1.86871300	-0.41390600
Si	-3.89550800	0.05328800	-3.12920600
Si	-3.88970800	-5.70681100	-1.77140700
Si	-5.80970600	-5.70891100	-0.41380500
Si	-3.89160800	-3.78681200	-3.12910700
Si	-0.05348600	-1.86280600	-1.77132300
Si	-1.97350800	-1.86441100	-0.41371100
Si	-0.05539000	0.05717500	-3.12913600
Si	-0.04956900	-5.70301900	-1.77134700
Si	-1.96981200	-5.70459900	-0.41391400
Si	-0.05150300	-3.78291200	-3.12912200
Si	3.77879300	5.82119300	-1.77140200
Si	1.85888700	5.81920900	-0.41390000
Si	3.78261000	1.98111100	-1.77126300
Si	1.86291300	1.97898000	-0.41397300
Si	3.78079900	3.90119300	-3.12909600
Si	5.69888800	5.82298500	-0.41379600
Si	5.70275500	1.98298300	-0.41376600
Si	3.78659300	-1.85908600	-1.77123300
Si	1.86658000	-1.86101600	-0.41413900
Si	3.78468300	0.06111700	-3.12916600
Si	3.79062500	-5.69919000	-1.77132400

Si	1.87047500	-5.70113300	-0.41383900
Si	3.78860300	-3.77901600	-3.12910400
Si	5.70651400	-1.85660000	-0.41356400
Si	5.71031900	-5.69682900	-0.41382600
H	-3.87190800	7.01058800	-2.68270700
H	-1.96400800	7.00288800	0.50729300
H	-7.13890800	2.00588800	-1.10570600
H	-0.06170600	7.07838600	-2.58311000
H	-7.06820800	5.49268800	-1.17220700
H	-5.95060800	7.06848800	0.38089300
H	-3.03670800	3.92108800	-4.33420700
H	-5.31150800	3.90588800	-3.66680700
H	1.11199200	3.85568800	-4.03180700
H	-1.23260800	3.84768800	-4.02840700
H	-3.04440800	0.06668800	-4.34610700
H	-5.31020800	0.06318800	-3.66690700
H	1.10969200	0.07268800	-4.04210700
H	-1.24310800	0.07098800	-4.01150700
H	1.11539200	-3.72371200	-4.03750700
H	-1.22670800	-3.71921200	-4.02550700
H	3.76869300	7.01708700	-2.68420900
H	5.79789600	7.05588700	0.42619300
H	6.96779100	5.54828400	-1.15070800
H	1.85138900	7.01399000	0.49549000
H	7.03299100	2.02487100	-1.08811000
H	5.19409200	3.90758800	-3.66480700

H	2.91849200	3.92828800	-4.33380700
H	7.03353800	-1.83392200	-1.09601200
H	5.19449200	0.07488800	-3.67830700
H	2.91859200	0.07728800	-4.33380700
H	1.86488000	-6.90168300	0.48483100
H	3.78329800	-6.88624500	-2.69626500
H	6.97002400	-5.40449300	-1.16131400
H	5.82023500	-6.93889400	0.40630100
H	5.20129200	-3.76881200	-3.66690700
H	2.92569200	-3.78781200	-4.33390700
H	-0.04559700	-6.95340000	-2.59952600
H	-5.91790700	-6.95391200	0.40189300
H	-7.06580900	-5.42011200	-1.16880600
H	-7.13310900	-1.83941200	-1.11080600
H	-3.87120800	-6.89221200	-2.69920700
H	-1.95060900	-6.90201300	0.48939200
H	-3.02940800	-3.79991200	-4.33510700
H	-5.30300800	-3.78971200	-3.67060700
Si	-5.14396300	0.05202800	0.79280700
Si	-5.10588300	3.90096800	0.83187800
Si	-2.64675400	3.89035300	0.80656600
Si	-5.09219100	-3.79469700	0.82791100
Si	-2.69007100	0.05811100	0.79905900
Si	-2.62348700	-3.77302900	0.80363700
Si	2.51639000	0.04676600	0.79910300
Si	2.54107300	3.89680500	0.82090400

Si	4.99360100	3.90622100	0.80830800
Si	2.54722400	-3.76875700	0.81443400
Si	4.98421700	0.05832700	0.80444500
Si	5.00819000	-3.78673500	0.82287800
S	-5.71278600	-3.70695100	2.90972000
S	-1.86135700	-3.68747800	2.84850800
S	1.86703600	-3.91401000	2.85483700
S	5.75037900	-3.97136400	2.83728300
S	-5.83306100	4.08159300	2.85308400
S	-1.85206400	4.06640700	2.81187300
S	2.12129700	3.92953500	2.93731500
S	5.73995600	3.73153900	2.83679300
S	-5.93595500	0.23776400	2.79372300
S	-2.25593600	0.09940900	2.93009000
S	1.69428200	0.06494700	2.80174400
S	5.65749500	-0.10306000	2.85406200
H	-4.50824000	-4.05539600	3.40467000
H	-1.30573200	-4.91151400	2.85053400
H	3.49602400	-3.00052500	5.36258100
H	5.15404200	-2.86093900	3.31317300
H	-5.23181400	2.97534600	3.33180000
H	-2.19605800	2.82513200	3.21109800
H	0.78007000	4.00473100	2.81669300
H	5.11926700	4.83077400	3.30439100
H	-5.57817500	-0.99339200	3.21066400
H	-0.92784000	0.30397700	2.78783500

H	4.90607000	0.91565200	3.31892000
Al	1.26019200	-1.94752400	3.61940900
C	0.30354000	-1.89321500	5.30180400
C	3.78454100	-2.01879000	5.74241000
H	0.65062200	-1.06638500	5.92627700
H	-0.76662500	-1.75365600	5.12369700
H	0.43159000	-2.82570200	5.85739600
H	4.83902000	-2.04318000	6.01782700
H	3.65260900	-1.24991800	4.97633300
H	3.18408000	-1.77080700	6.61690100
P^{A2-d}			
Si	-3.90130000	5.81340000	-1.77140000
Si	-5.82130000	5.81150000	-0.41380000
Si	-3.89750000	1.97330000	-1.77130000
Si	-5.81750000	1.97120000	-0.41370000
Si	-3.89940000	3.89340000	-3.12910000
Si	-0.06140000	5.81740000	-1.77140000
Si	-1.98130000	5.81530000	-0.41380000
Si	-0.05750000	1.97720000	-1.77130000
Si	-1.97730000	1.97520000	-0.41390000
Si	-0.05930000	3.89730000	-3.12910000
Si	-3.89370000	-1.86680000	-1.77130000
Si	-5.81360000	-1.86870000	-0.41390000
Si	-3.89550000	0.05330000	-3.12920000
Si	-3.88970000	-5.70680000	-1.77140000

Si	-5.80970000	-5.70890000	-0.41380000
Si	-3.89160000	-3.78680000	-3.12910000
Si	-0.05350000	-1.86280000	-1.77130000
Si	-1.97350000	-1.86440000	-0.41370000
Si	-0.05540000	0.05720000	-3.12910000
Si	-0.04960000	-5.70300000	-1.77130000
Si	-1.96980000	-5.70460000	-0.41390000
Si	-0.05150000	-3.78290000	-3.12910000
Si	3.77880000	5.82120000	-1.77140000
Si	1.85890000	5.81920000	-0.41390000
Si	3.78260000	1.98110000	-1.77130000
Si	1.86290000	1.97900000	-0.41400000
Si	3.78080000	3.90120000	-3.12910000
Si	5.69890000	5.82300000	-0.41380000
Si	5.70280000	1.98300000	-0.41380000
Si	3.78660000	-1.85910000	-1.77120000
Si	1.86660000	-1.86100000	-0.41410000
Si	3.78470000	0.06110000	-3.12920000
Si	3.79060000	-5.69920000	-1.77130000
Si	1.87050000	-5.70110000	-0.41380000
Si	3.78860000	-3.77900000	-3.12910000
Si	5.70650000	-1.85660000	-0.41360000
Si	5.71030000	-5.69680000	-0.41380000
H	-3.87190000	7.01060000	-2.68270000
H	-1.96400000	7.00290000	0.50730000
H	-7.13890000	2.00590000	-1.10570000

H	-0.06170000	7.07840000	-2.58310000
H	-7.06820000	5.49270000	-1.17220000
H	-5.95060000	7.06850000	0.38090000
H	-3.03670000	3.92110000	-4.33420000
H	-5.31150000	3.90590000	-3.66680000
H	1.11200000	3.85570000	-4.03180000
H	-1.23260000	3.84770000	-4.02840000
H	-3.04440000	0.06670000	-4.34610000
H	-5.31020000	0.06320000	-3.66690000
H	1.10970000	0.07270000	-4.04210000
H	-1.24310000	0.07100000	-4.01150000
H	1.11540000	-3.72370000	-4.03750000
H	-1.22670000	-3.71920000	-4.02550000
H	3.76870000	7.01710000	-2.68420000
H	5.79790000	7.05590000	0.42620000
H	6.96780000	5.54830000	-1.15070000
H	1.85140000	7.01400000	0.49550000
H	7.03300000	2.02490000	-1.08810000
H	5.19410000	3.90760000	-3.66480000
H	2.91850000	3.92830000	-4.33380000
H	7.03350000	-1.83390000	-1.09600000
H	5.19450000	0.07490000	-3.67830000
H	2.91860000	0.07730000	-4.33380000
H	1.86490000	-6.90170000	0.48480000
H	3.78330000	-6.88620000	-2.69630000
H	6.97000000	-5.40450000	-1.16130000

H	5.82020000	-6.93890000	0.40630000
H	5.20130000	-3.76880000	-3.66690000
H	2.92570000	-3.78780000	-4.33390000
H	-0.04560000	-6.95340000	-2.59950000
H	-5.91790000	-6.95390000	0.40190000
H	-7.06580000	-5.42010000	-1.16880000
H	-7.13310000	-1.83940000	-1.11080000
H	-3.87120000	-6.89220000	-2.69920000
H	-1.95060000	-6.90200000	0.48940000
H	-3.02940000	-3.79990000	-4.33510000
H	-5.30300000	-3.78970000	-3.67060000
Si	-5.14571200	0.05200800	0.79227500
Si	-5.10603700	3.90091400	0.83203700
Si	-2.64705400	3.89058400	0.80664300
Si	-5.09086400	-3.79469000	0.82911900
Si	-2.69264900	0.05914300	0.79745600
Si	-2.62174900	-3.77172900	0.80254200
Si	2.51117600	0.04657800	0.79919500
Si	2.54143200	3.89667300	0.82062900
Si	4.99408800	3.90624100	0.80816000
Si	2.55273700	-3.76852900	0.81669400
Si	4.98071300	0.05740300	0.80793900
Si	5.01330400	-3.78782000	0.82118900
S	-5.70757200	-3.70673500	2.91229900
S	-1.84516400	-3.67141500	2.84391400
S	1.90298000	-3.90746000	2.86995900

S	5.77195500	-3.98600700	2.82631400
S	-5.83301000	4.08037400	2.85337900
S	-1.85302000	4.07070900	2.81176900
S	2.12284700	3.92461100	2.93735000
S	5.74039900	3.72903900	2.83611600
S	-5.93921300	0.23702700	2.79250600
S	-2.26456200	0.10962900	2.92895500
S	1.66867900	0.05654100	2.79494800
S	5.64286700	-0.11197000	2.86025900
H	-4.50205800	-4.05244800	3.40637500
H	-1.29200000	-4.89682300	2.85170000
H	5.17839400	-2.88110200	3.31635600
H	-5.23178500	2.97370700	3.33120800
H	-2.20684400	2.83417900	3.21675700
H	0.78119700	3.99473600	2.81839400
H	5.12008000	4.82792200	3.30507800
H	-5.58084900	-0.99376500	3.20994900
H	-0.93857100	0.32918700	2.78899500
H	4.88548800	0.90196100	3.32517800
Al	1.20406700	-1.95802700	3.58647400
C	0.26623300	-1.91720600	5.28006400
H	0.76433400	-1.25842000	5.99574700
H	-0.75285100	-1.54602600	5.13897300
H	0.19989000	-2.91626000	5.71694100

P^{A2-a}

Si	-3.84640000	5.74340000	-1.76960000
Si	-5.76640000	5.74150000	-0.41200000
Si	-3.84260000	1.90330000	-1.76950000
Si	-5.76260000	1.90120000	-0.41190000
Si	-3.84450000	3.82340000	-3.12730000
Si	-0.00650000	5.74740000	-1.76960000
Si	-1.92640000	5.74530000	-0.41200000
Si	-0.00270000	1.90720000	-1.76950000
Si	-1.92250000	1.90530000	-0.41210000
Si	-0.00440000	3.82730000	-3.12730000
Si	-3.83880000	-1.93680000	-1.76950000
Si	-5.75870000	-1.93870000	-0.41210000
Si	-3.84060000	-0.01670000	-3.12740000
Si	-3.83480000	-5.77680000	-1.76960000
Si	-5.75480000	-5.77890000	-0.41200000
Si	-3.83670000	-3.85680000	-3.12730000
Si	0.00140000	-1.93280000	-1.76950000
Si	-1.91860000	-1.93430000	-0.41190000
Si	-0.00050000	-0.01280000	-3.12730000
Si	0.00530000	-5.77300000	-1.76950000
Si	-1.91490000	-5.77460000	-0.41210000
Si	0.00340000	-3.85290000	-3.12730000
Si	3.83370000	5.75120000	-1.76960000
Si	1.91380000	5.74920000	-0.41210000
Si	3.83750000	1.91110000	-1.76950000

Si	1.91780000	1.90880000	-0.41220000
Si	3.83570000	3.83120000	-3.12730000
Si	5.75380000	5.75300000	-0.41200000
Si	5.75770000	1.91300000	-0.41200000
Si	3.84150000	-1.92910000	-1.76950000
Si	1.92160000	-1.93100000	-0.41230000
Si	3.83960000	-0.00890000	-3.12740000
Si	3.84550000	-5.76910000	-1.76960000
Si	1.92540000	-5.77110000	-0.41210000
Si	3.84350000	-3.84900000	-3.12730000
Si	5.76150000	-1.92660000	-0.41170000
Si	5.76520000	-5.76680000	-0.41200000
H	-3.81700000	6.94060000	-2.68090000
H	-1.90910000	6.93290000	0.50910000
H	-7.08400000	1.93590000	-1.10390000
H	-0.00680000	7.00840000	-2.58130000
H	-7.01330000	5.42270000	-1.17040000
H	-5.89570000	6.99850000	0.38270000
H	-2.98180000	3.85110000	-4.33240000
H	-5.25660000	3.83590000	-3.66500000
H	1.16690000	3.78570000	-4.03000000
H	-1.17770000	3.77770000	-4.02660000
H	-2.98950000	-0.00330000	-4.34430000
H	-5.25530000	-0.00680000	-3.66510000
H	1.16460000	0.00270000	-4.04030000
H	-1.18820000	0.00100000	-4.00970000

H	1.17030000	-3.79370000	-4.03570000
H	-1.17180000	-3.78920000	-4.02370000
H	3.82360000	6.94710000	-2.68240000
H	5.85280000	6.98590000	0.42800000
H	7.02270000	5.47830000	-1.14890000
H	1.90630000	6.94400000	0.49730000
H	7.08790000	1.95490000	-1.08630000
H	5.24900000	3.83760000	-3.66300000
H	2.97340000	3.85830000	-4.33200000
H	7.08850000	-1.90390000	-1.09410000
H	5.24940000	0.00490000	-3.67650000
H	2.97350000	0.00730000	-4.33200000
H	1.91990000	-6.97170000	0.48660000
H	3.83820000	-6.95620000	-2.69450000
H	7.02500000	-5.47450000	-1.15940000
H	5.87500000	-7.00890000	0.40810000
H	5.25620000	-3.83880000	-3.66510000
H	2.98060000	-3.85780000	-4.33210000
H	0.00930000	-7.02340000	-2.59770000
H	-5.86300000	-7.02390000	0.40370000
H	-7.01090000	-5.49010000	-1.16700000
H	-7.07820000	-1.90940000	-1.10900000
H	-3.81630000	-6.96220000	-2.69740000
H	-1.89570000	-6.97200000	0.49120000
H	-2.97450000	-3.86990000	-4.33330000
H	-5.24810000	-3.85970000	-3.66880000

Si	-5.02723800	-0.01933900	0.80834600
Si	-5.06977700	3.83104900	0.82960200
Si	-2.61127600	3.81947400	0.80862200
Si	-5.05130300	-3.86364200	0.81162700
Si	-2.54159300	-0.00475900	0.81737900
Si	-2.59523300	-3.85159000	0.82068300
Si	2.57589500	-0.00560800	0.80605300
Si	2.57845200	3.81670000	0.80388400
Si	5.03714500	3.83212000	0.82314800
Si	2.59440200	-3.84377100	0.80847900
Si	5.04773100	-0.01343300	0.80175700
Si	5.05710200	-3.85809100	0.83121900
S	-5.77761200	-3.69062800	2.84718700
S	-2.16605100	-3.88758600	2.93587200
S	1.79044700	-3.97332800	2.81502700
S	5.78898500	-4.06172000	2.84617900
S	-5.83122800	4.01332500	2.83781600
S	-1.89667700	4.00734700	2.84580700
S	1.84445800	3.75081800	2.86530300
S	5.68789600	3.64998500	2.88156700
S	-5.75590200	0.13833500	2.84025200
S	-1.94211100	0.14340900	2.88609600
S	2.05247100	0.01749300	2.90276600
S	5.75438800	-0.19502600	2.83426200
H	-5.05348900	-4.71976700	3.32536400
H	-0.83580600	-4.07021800	2.80802800

H	1.95137500	-2.66863000	3.11781200
H	5.19546000	-2.95544200	3.33382300
H	-5.49148700	2.77458500	3.24549800
H	-2.62589900	2.98919800	3.34258900
H	1.02468000	4.80922600	2.75345600
H	4.87527700	4.61494300	3.35301100
H	-4.98328700	-0.84650600	3.33973100
H	4.99711100	0.80630300	3.32422300
Al	0.07716800	0.87581200	3.46260800
C	0.05908900	1.69671100	5.21789300
H	1.07588800	1.83928600	5.58953800
H	-0.43254700	2.67210300	5.19004400
H	-0.48909500	1.07027300	5.92718000
Im1 ^{B1-I}			
Si	-3.84550400	5.87973400	-1.91672300
Si	-5.76550400	5.87783400	-0.55912300
Si	-3.84170400	2.03963400	-1.91662300
Si	-5.76170400	2.03753400	-0.55902300
Si	-3.84360400	3.95973400	-3.27442300
Si	-0.00560400	5.88373400	-1.91672300
Si	-1.92550400	5.88163400	-0.55912300
Si	-0.00180400	2.04353400	-1.91662300
Si	-1.92160400	2.04163400	-0.55922300
Si	-0.00350400	3.96363400	-3.27442300
Si	-3.83790400	-1.80046600	-1.91662300

Si	-5.75780400	-1.80236600	-0.55922300
Si	-3.83970400	0.11963400	-3.27452300
Si	-3.83390400	-5.64046600	-1.91672300
Si	-5.75390400	-5.64256600	-0.55912300
Si	-3.83580400	-3.72046600	-3.27442300
Si	0.00239600	-1.79646600	-1.91672300
Si	-1.91770400	-1.79796600	-0.55902300
Si	0.00039600	0.12353400	-3.27442300
Si	0.00629600	-5.63666600	-1.91672300
Si	-1.91400400	-5.63826600	-0.55922300
Si	0.00429600	-3.71656600	-3.27442300
Si	3.83459600	5.88753400	-1.91672300
Si	1.91469600	5.88553400	-0.55922300
Si	3.83839600	2.04743400	-1.91662300
Si	1.91869600	2.04513400	-0.55932300
Si	3.83659600	3.96753400	-3.27442300
Si	5.75469600	5.88933400	-0.55912300
Si	5.75859600	2.04933400	-0.55912300
Si	3.84249600	-1.79276600	-1.91652300
Si	1.92239600	-1.79456600	-0.55942300
Si	3.84049600	0.12743400	-3.27452300
Si	3.84639600	-5.63276600	-1.91672300
Si	1.92629600	-5.63486600	-0.55912300
Si	3.84439600	-3.71266600	-3.27442300
Si	5.76229600	-1.79036600	-0.55892300
Si	5.76599600	-5.63046600	-0.55912300

H	-3.81610400	7.07693400	-2.82802300
H	-1.90820400	7.06923400	0.36197700
H	-7.08310400	2.07223400	-1.25102300
H	-0.00590400	7.14473400	-2.72842300
H	-7.01240400	5.55903400	-1.31752300
H	-5.89480400	7.13483400	0.23557700
H	-2.98090400	3.98743400	-4.47952300
H	-5.25570400	3.97223400	-3.81212300
H	1.16779600	3.92203400	-4.17712300
H	-1.17680400	3.91403400	-4.17372300
H	-2.98860400	0.13303400	-4.49142300
H	-5.25440400	0.12953400	-3.81222300
H	1.16549600	0.13903400	-4.18742300
H	-1.18730400	0.13733400	-4.15682300
H	1.17119600	-3.65736600	-4.18282300
H	-1.17090400	-3.65286600	-4.17082300
H	3.82449600	7.08343400	-2.82952300
H	5.85369600	7.12223400	0.28087700
H	7.02359600	5.61463400	-1.29602300
H	1.90719600	7.08033400	0.35017700
H	7.08879600	2.09123400	-1.23342300
H	5.24989600	3.97393400	-3.81012300
H	2.97429600	3.99463400	-4.47912300
H	7.08939600	-1.76756600	-1.24122300
H	5.25029600	0.14123400	-3.82362300
H	2.97439600	0.14363400	-4.47912300

H	1.92069600	-6.83536600	0.33947700
H	3.83909600	-6.81986600	-2.84162300
H	7.02589600	-5.33816600	-1.30652300
H	5.87589600	-6.87256600	0.26097700
H	5.25709600	-3.70246600	-3.81222300
H	2.98149600	-3.72146600	-4.47922300
H	0.01019600	-6.88706600	-2.74482300
H	-5.86210400	-6.88756600	0.25657700
H	-7.01000400	-5.35376600	-1.31412300
H	-7.07730400	-1.77306600	-1.25612300
H	-3.81540400	-6.82586600	-2.84452300
H	-1.89480400	-6.83566600	0.34407700
H	-2.97360400	-3.73356600	-4.48042300
H	-5.24720400	-3.72336600	-3.81592300
Si	-5.04311800	0.11940900	0.65380400
Si	-5.05763800	3.96814800	0.68550700
Si	-2.59922100	3.95665700	0.65896600
Si	-5.05090700	-3.72414200	0.66753400
Si	-2.56586500	0.12688300	0.66912400
Si	-2.59673300	-3.71832500	0.66066300
Si	2.56372100	0.12460900	0.67152500
Si	2.59459700	3.96356100	0.66810100
Si	5.04581600	3.97024600	0.66522000
Si	2.60622200	-3.70794800	0.65143300
Si	5.04051400	0.12633900	0.65529300
Si	5.06665700	-3.72066800	0.68269000

S	-5.73283600	-3.54875600	2.71803400
S	-2.09721600	-3.90192700	2.77645400
S	1.82098000	-3.88220200	2.66540400
S	5.80292600	-3.91435500	2.69797800
S	-5.79981600	4.15338800	2.69954500
S	-1.82162200	4.14853200	2.67005800
S	2.12723600	4.00918000	2.77963400
S	5.76134700	3.78930300	2.70353100
S	-5.79485700	0.27842200	2.67608900
S	-2.07168000	0.19348500	2.75621200
S	2.06756900	0.00058300	2.75975000
S	5.77092000	-0.03312300	2.68482900
H	-4.98528000	-4.56740100	3.18350600
H	-0.93690900	-4.55751300	2.59518900
H	2.17951500	-2.63880000	3.05153500
H	5.38885000	-2.70454600	3.12454200
H	-5.37063200	2.94859100	3.12524100
H	-2.19893300	2.92378500	3.09210500
H	0.82711700	4.33042300	2.62433400
H	5.12283600	4.88038300	3.16616500
H	-5.02851100	-0.70878700	3.17882600
H	4.98546000	0.93994800	3.18763000
Al	0.02492400	0.50877800	3.54148100
C	0.00680600	1.82468900	4.97727400
H	0.85840000	1.66632800	5.64601700
H	0.08123400	2.84905300	4.60790700

H	-0.91317300	1.75450200	5.56680600
S	-0.05114500	-1.57014100	4.98700600
H	-0.68440600	-2.35988600	4.08426100
H	-1.19688600	-1.26442300	5.62393900
S	0.12015000	-5.38276900	5.65355500
H	0.90673100	-6.00255500	4.76057200
H	1.09112400	-4.51709700	5.98278000
TS ^{B1-I}			
Si	-3.84640000	5.74340000	-1.76960000
Si	-5.76640000	5.74150000	-0.41200000
Si	-3.84260000	1.90330000	-1.76950000
Si	-5.76260000	1.90120000	-0.41190000
Si	-3.84450000	3.82340000	-3.12730000
Si	-0.00650000	5.74740000	-1.76960000
Si	-1.92640000	5.74530000	-0.41200000
Si	-0.00270000	1.90720000	-1.76950000
Si	-1.92250000	1.90530000	-0.41210000
Si	-0.00440000	3.82730000	-3.12730000
Si	-3.83880000	-1.93680000	-1.76950000
Si	-5.75870000	-1.93870000	-0.41210000
Si	-3.84060000	-0.01670000	-3.12740000
Si	-3.83480000	-5.77680000	-1.76960000
Si	-5.75480000	-5.77890000	-0.41200000
Si	-3.83670000	-3.85680000	-3.12730000
Si	0.00150000	-1.93280000	-1.76960000

Si	-1.91860000	-1.93430000	-0.41190000
Si	-0.00050000	-0.01280000	-3.12730000
Si	0.00540000	-5.77300000	-1.76960000
Si	-1.91490000	-5.77460000	-0.41210000
Si	0.00340000	-3.85290000	-3.12730000
Si	3.83370000	5.75120000	-1.76960000
Si	1.91380000	5.74920000	-0.41210000
Si	3.83750000	1.91110000	-1.76950000
Si	1.91780000	1.90880000	-0.41220000
Si	3.83570000	3.83120000	-3.12730000
Si	5.75380000	5.75300000	-0.41200000
Si	5.75770000	1.91300000	-0.41200000
Si	3.84160000	-1.92910000	-1.76940000
Si	1.92150000	-1.93090000	-0.41230000
Si	3.83960000	-0.00890000	-3.12740000
Si	3.84550000	-5.76910000	-1.76960000
Si	1.92540000	-5.77120000	-0.41200000
Si	3.84350000	-3.84900000	-3.12730000
Si	5.76140000	-1.92670000	-0.41180000
Si	5.76510000	-5.76680000	-0.41200000
H	-3.81700000	6.94060000	-2.68090000
H	-1.90910000	6.93290000	0.50910000
H	-7.08400000	1.93590000	-1.10390000
H	-0.00680000	7.00840000	-2.58130000
H	-7.01330000	5.42270000	-1.17040000
H	-5.89570000	6.99850000	0.38270000

H	-2.98180000	3.85110000	-4.33240000
H	-5.25660000	3.83590000	-3.66500000
H	1.16690000	3.78570000	-4.03000000
H	-1.17770000	3.77770000	-4.02660000
H	-2.98950000	-0.00330000	-4.34430000
H	-5.25530000	-0.00680000	-3.66510000
H	1.16460000	0.00270000	-4.04030000
H	-1.18820000	0.00100000	-4.00970000
H	1.17030000	-3.79370000	-4.03570000
H	-1.17180000	-3.78920000	-4.02370000
H	3.82360000	6.94710000	-2.68240000
H	5.85280000	6.98590000	0.42800000
H	7.02270000	5.47830000	-1.14890000
H	1.90630000	6.94400000	0.49730000
H	7.08790000	1.95490000	-1.08630000
H	5.24900000	3.83760000	-3.66300000
H	2.97340000	3.85830000	-4.33200000
H	7.08850000	-1.90390000	-1.09410000
H	5.24940000	0.00490000	-3.67650000
H	2.97350000	0.00730000	-4.33200000
H	1.91980000	-6.97170000	0.48660000
H	3.83820000	-6.95620000	-2.69450000
H	7.02500000	-5.47450000	-1.15940000
H	5.87500000	-7.00890000	0.40810000
H	5.25620000	-3.83880000	-3.66510000
H	2.98060000	-3.85780000	-4.33210000

H	0.00930000	-7.02340000	-2.59770000
H	-5.86300000	-7.02390000	0.40370000
H	-7.01090000	-5.49010000	-1.16700000
H	-7.07820000	-1.90940000	-1.10900000
H	-3.81630000	-6.96220000	-2.69740000
H	-1.89570000	-6.97200000	0.49120000
H	-2.97450000	-3.86990000	-4.33330000
H	-5.24810000	-3.85970000	-3.66880000
Si	-5.05232700	-0.01771900	0.80008000
Si	-5.05819600	3.83176700	0.83332700
Si	-2.59859500	3.82160100	0.80847400
Si	-5.05056600	-3.86253600	0.81431900
Si	-2.58039900	-0.01046400	0.80086700
Si	-2.59573600	-3.85158200	0.81797700
Si	2.58051500	-0.01392000	0.80572500
Si	2.59042600	3.82727700	0.81724500
Si	5.04309100	3.83452000	0.81463100
Si	2.60281900	-3.84604800	0.79902000
Si	5.05294300	-0.01094900	0.80238200
Si	5.06187700	-3.85693800	0.83029300
S	-5.75487800	-3.69152600	2.85818100
S	-2.13664800	-3.92019400	2.93277400
S	1.80002200	-4.01198300	2.80244200
S	5.78232200	-4.04783000	2.85134800
S	-5.80286700	4.01661000	2.84671400
S	-1.82682600	4.03706300	2.82171800

S	2.10290100	3.90005300	2.92855200
S	5.74085900	3.66369600	2.86115500
S	-5.78720000	0.13902500	2.82806600
S	-2.09519100	0.13603200	2.90052400
S	2.11825400	-0.09448700	2.91552000
S	5.78207800	-0.17980300	2.82894800
H	-5.02083600	-4.71777400	3.32825300
H	-0.84218500	-4.26968100	2.79318000
H	2.10815700	-2.75644500	3.18663000
H	5.19279600	-2.93257100	3.32404000
H	-5.37525800	2.81188300	3.27385300
H	-2.19177600	2.80981600	3.24557400
H	0.82105500	4.27852100	2.75773900
H	4.99722000	4.68191900	3.33336900
H	-5.04100700	-0.87054100	3.31728000
H	5.05584800	0.84561500	3.31560900
Al	0.00915800	-0.02595700	3.57787100
C	0.02414700	1.32468300	5.14371400
H	0.87369100	1.41398000	5.82480100
H	0.17798200	2.12918500	4.40391200
H	-0.90423500	1.56253300	5.66725100
S	-0.08217700	-1.77885100	5.21635200
H	-1.42458500	-1.84154900	5.14101100
H	-0.05649300	-0.20120100	5.43626500
S	0.11389400	-6.00682300	5.49812400
H	1.36538800	-6.04949100	5.01481400

H	0.12856100	-4.66405000	5.53935600
Im2 ^{B1-I}			
Si	-3.84550400	5.87973400	-1.91672300
Si	-5.76550400	5.87783400	-0.55912300
Si	-3.84170400	2.03963400	-1.91662300
Si	-5.76170400	2.03753400	-0.55902300
Si	-3.84360400	3.95973400	-3.27442300
Si	-0.00560400	5.88373400	-1.91672300
Si	-1.92550400	5.88163400	-0.55912300
Si	-0.00180400	2.04353400	-1.91662300
Si	-1.92160400	2.04163400	-0.55922300
Si	-0.00350400	3.96363400	-3.27442300
Si	-3.83790400	-1.80046600	-1.91662300
Si	-5.75780400	-1.80236600	-0.55922300
Si	-3.83970400	0.11963400	-3.27452300
Si	-3.83390400	-5.64046600	-1.91672300
Si	-5.75390400	-5.64256600	-0.55912300
Si	-3.83580400	-3.72046600	-3.27442300
Si	0.00239600	-1.79646600	-1.91672300
Si	-1.91770400	-1.79796600	-0.55902300
Si	0.00039600	0.12353400	-3.27442300
Si	0.00629600	-5.63666600	-1.91672300
Si	-1.91400400	-5.63826600	-0.55922300
Si	0.00429600	-3.71656600	-3.27442300
Si	3.83459600	5.88753400	-1.91672300

Si	1.91469600	5.88553400	-0.55922300
Si	3.83839600	2.04743400	-1.91662300
Si	1.91869600	2.04513400	-0.55932300
Si	3.83659600	3.96753400	-3.27442300
Si	5.75469600	5.88933400	-0.55912300
Si	5.75859600	2.04933400	-0.55912300
Si	3.84249600	-1.79276600	-1.91652300
Si	1.92239600	-1.79456600	-0.55942300
Si	3.84049600	0.12743400	-3.27452300
Si	3.84639600	-5.63276600	-1.91672300
Si	1.92629600	-5.63486600	-0.55912300
Si	3.84439600	-3.71266600	-3.27442300
Si	5.76229600	-1.79036600	-0.55892300
Si	5.76599600	-5.63046600	-0.55912300
H	-3.81610400	7.07693400	-2.82802300
H	-1.90820400	7.06923400	0.36197700
H	-7.08310400	2.07223400	-1.25102300
H	-0.00590400	7.14473400	-2.72842300
H	-7.01240400	5.55903400	-1.31752300
H	-5.89480400	7.13483400	0.23557700
H	-2.98090400	3.98743400	-4.47952300
H	-5.25570400	3.97223400	-3.81212300
H	1.16779600	3.92203400	-4.17712300
H	-1.17680400	3.91403400	-4.17372300
H	-2.98860400	0.13303400	-4.49142300
H	-5.25440400	0.12953400	-3.81222300

H	1.16549600	0.13903400	-4.18742300
H	-1.18730400	0.13733400	-4.15682300
H	1.17119600	-3.65736600	-4.18282300
H	-1.17090400	-3.65286600	-4.17082300
H	3.82449600	7.08343400	-2.82952300
H	5.85369600	7.12223400	0.28087700
H	7.02359600	5.61463400	-1.29602300
H	1.90719600	7.08033400	0.35017700
H	7.08879600	2.09123400	-1.23342300
H	5.24989600	3.97393400	-3.81012300
H	2.97429600	3.99463400	-4.47912300
H	7.08939600	-1.76756600	-1.24122300
H	5.25029600	0.14123400	-3.82362300
H	2.97439600	0.14363400	-4.47912300
H	1.92069600	-6.83536600	0.33947700
H	3.83909600	-6.81986600	-2.84162300
H	7.02589600	-5.33816600	-1.30652300
H	5.87589600	-6.87256600	0.26097700
H	5.25709600	-3.70246600	-3.81222300
H	2.98149600	-3.72146600	-4.47922300
H	0.01019600	-6.88706600	-2.74482300
H	-5.86210400	-6.88756600	0.25657700
H	-7.01000400	-5.35376600	-1.31412300
H	-7.07730400	-1.77306600	-1.25612300
H	-3.81540400	-6.82586600	-2.84452300
H	-1.89480400	-6.83566600	0.34407700

H	-2.97360400	-3.73356600	-4.48042300
H	-5.24720400	-3.72336600	-3.81592300
Si	-5.05255500	0.12189700	0.65581500
Si	-5.05116900	3.96949500	0.68735600
Si	-2.59096900	3.95648500	0.66174300
Si	-5.04644500	-3.72352700	0.66897500
Si	-2.58129900	0.11998300	0.64743300
Si	-2.58976100	-3.71475400	0.66516800
Si	2.56187900	0.12012800	0.65813700
Si	2.59535500	3.96498100	0.67264100
Si	5.04763600	3.97203000	0.66461700
Si	2.61437700	-3.70816600	0.65591900
Si	5.04119700	0.12849400	0.66022700
Si	5.07276700	-3.72023800	0.68220800
S	-5.72111500	-3.53224500	2.71826400
S	-2.02137500	-3.74664100	2.76335900
S	1.84203900	-3.88608100	2.66962900
S	5.81782100	-3.91050400	2.69439400
S	-5.77888900	4.17130400	2.70456300
S	-1.78480000	4.11244200	2.66530700
S	2.16612200	4.01517600	2.78848100
S	5.76879900	3.79923000	2.70240300
S	-5.75417200	0.30933800	2.68950600
S	-2.05894100	0.15724500	2.75794100
S	2.01709100	0.02087100	2.75825100
S	5.76287000	-0.02959600	2.69230100

H	-4.93633800	-4.51569000	3.19881100
H	-0.98053600	-4.58697200	2.63558400
H	2.45511900	-2.79321100	3.16568400
H	5.43251200	-2.69083100	3.11869500
H	-5.18161400	3.06651500	3.19090800
H	-1.96736000	2.81937800	3.00094600
H	0.84216200	4.24707000	2.66697300
H	5.04700100	4.82978700	3.18087300
H	-5.02764300	-0.71738900	3.17256400
H	5.01597100	0.97884300	3.18382400
Al	-0.03933700	-0.53076100	3.29742700
C	-0.11710700	2.31616700	5.23194100
H	0.52108300	1.78453200	5.93678300
H	0.30367200	2.23004200	4.22713200
H	-0.15885500	3.37319600	5.49716800
S	0.00253400	-1.51835900	5.24463500
H	-1.33416300	-1.67378800	5.28303700
H	-1.12383700	1.89626000	5.26506700
S	0.01479900	-5.65048700	5.39698900
H	1.28350500	-5.83502400	5.00128600
H	0.14787700	-4.31111300	5.38560000
Im1 ^{B1-II}			
Si	-3.77765600	5.79925700	-1.92284800
Si	-5.69765600	5.79735700	-0.56524800
Si	-3.77385600	1.95915700	-1.92274800

Si	-5.69385600	1.95705700	-0.56514800
Si	-3.77575600	3.87925700	-3.28054800
Si	0.06224400	5.80325700	-1.92284800
Si	-1.85765600	5.80115700	-0.56524800
Si	0.06604400	1.96305700	-1.92274800
Si	-1.85375600	1.96115700	-0.56534800
Si	0.06434400	3.88315700	-3.28054800
Si	-3.77005600	-1.88094300	-1.92274800
Si	-5.68995600	-1.88284300	-0.56534800
Si	-3.77185600	0.03915700	-3.28064800
Si	-3.76605600	-5.72094300	-1.92284800
Si	-5.68605600	-5.72304300	-0.56524800
Si	-3.76795600	-3.80094300	-3.28054800
Si	0.07014400	-1.87694300	-1.92274800
Si	-1.84985600	-1.87844300	-0.56514800
Si	0.06824400	0.04305700	-3.28054800
Si	0.07404400	-5.71714300	-1.92274800
Si	-1.84615600	-5.71874300	-0.56534800
Si	0.07214400	-3.79704300	-3.28054800
Si	3.90244400	5.80705700	-1.92284800
Si	1.98254400	5.80505700	-0.56534800
Si	3.90624400	1.96695700	-1.92274800
Si	1.98654400	1.96465700	-0.56544800
Si	3.90444400	3.88705700	-3.28054800
Si	5.82254400	5.80885700	-0.56524800
Si	5.82644400	1.96885700	-0.56524800

Si	3.91024400	-1.87324300	-1.92274800
Si	1.99034400	-1.87514300	-0.56554800
Si	3.90834400	0.04695700	-3.28064800
Si	3.91424400	-5.71324300	-1.92284800
Si	1.99414400	-5.71524300	-0.56534800
Si	3.91224400	-3.79314300	-3.28054800
Si	5.83024400	-1.87074300	-0.56494800
Si	5.83394400	-5.71094300	-0.56524800
H	-3.74825600	6.99645700	-2.83414800
H	-1.84035600	6.98875700	0.35585200
H	-7.01525600	1.99175700	-1.25714800
H	0.06194400	7.06425700	-2.73454800
H	-6.94455600	5.47855700	-1.32364800
H	-5.82695600	7.05435700	0.22945200
H	-2.91305600	3.90695700	-4.48564800
H	-5.18785600	3.89175700	-3.81824800
H	1.23564400	3.84155700	-4.18324800
H	-1.10895600	3.83355700	-4.17984800
H	-2.92075600	0.05255700	-4.49754800
H	-5.18655600	0.04905700	-3.81834800
H	1.23334400	0.05855700	-4.19354800
H	-1.11945600	0.05685700	-4.16294800
H	1.23904400	-3.73784300	-4.18894800
H	-1.10305600	-3.73334300	-4.17694800
H	3.89234400	7.00295700	-2.83564800
H	5.92154400	7.04175700	0.27475200

H	7.09144400	5.53415700	-1.30214800
H	1.97504400	6.99985700	0.34405200
H	7.15664400	2.01075700	-1.23954800
H	5.31774400	3.89345700	-3.81624800
H	3.04214400	3.91415700	-4.48524800
H	7.15724400	-1.84804300	-1.24734800
H	5.31814400	0.06075700	-3.82974800
H	3.04224400	0.06315700	-4.48524800
H	1.98864400	-6.91584300	0.33335200
H	3.90694400	-6.90034300	-2.84774800
H	7.09374400	-5.41864300	-1.31264800
H	5.94374400	-6.95304300	0.25485200
H	5.32494400	-3.78294300	-3.81834800
H	3.04934400	-3.80194300	-4.48534800
H	0.07804400	-6.96754300	-2.75094800
H	-5.79425600	-6.96804300	0.25045200
H	-6.94215600	-5.43424300	-1.32024800
H	-7.00945600	-1.85354300	-1.26224800
H	-3.74755600	-6.90634300	-2.85064800
H	-1.82695600	-6.91614300	0.33795200
H	-2.90575600	-3.81404300	-4.48654800
H	-5.17935600	-3.80384300	-3.82204800
Si	-4.98109400	0.04048000	0.64522000
Si	-4.98646100	3.88677300	0.67792600
Si	-2.52919100	3.87696700	0.65200500
Si	-4.97827200	-3.80738800	0.65800400

Si	-2.50375900	0.04651300	0.66112500
Si	-2.52449700	-3.79517200	0.66070000
Si	2.63699400	0.04416600	0.66346900
Si	2.65939200	3.88220300	0.66320800
Si	5.11220000	3.89027400	0.66067500
Si	2.66714800	-3.79190000	0.64586700
Si	5.11290400	0.04421100	0.65016800
Si	5.12801300	-3.80109000	0.67536900
S	-5.68510900	-3.63321500	2.70532500
S	-2.06720100	-3.86725000	2.78236300
S	1.86917100	-3.95422700	2.65192400
S	5.85304900	-3.99223900	2.69463400
S	-5.71655800	4.06426100	2.69830700
S	-1.75769600	4.07130300	2.66552200
S	2.17968400	3.92550700	2.77408800
S	5.81198900	3.72111900	2.70655100
S	-5.77271800	0.20896800	2.65242100
S	-2.00728500	0.14764100	2.75094600
S	2.14708500	-0.05866200	2.75684100
S	5.83706500	-0.12317000	2.67928800
H	-5.06530000	-4.73960300	3.15790500
H	-0.73771500	-4.06595100	2.65283300
H	2.07555500	-2.65736100	2.96221100
H	5.26385800	-2.87695600	3.16759900
H	-5.12133700	2.95088200	3.16792100
H	-2.09074200	2.82713600	3.06792200

H	0.88417600	4.26150700	2.61439300
H	5.07082300	4.74162500	3.17763100
H	-5.17733600	-0.90325500	3.12350000
H	5.07907400	0.87833000	3.16820700
Al	0.09432700	0.39056800	3.54100100
C	0.08125500	1.68693400	4.99660200
H	0.99971900	1.61088000	5.58693600
H	0.02366300	2.71665700	4.63677900
H	-0.77279300	1.52161000	5.66223900
S	-0.00524700	-1.74548600	4.90886500
H	-1.26872700	-1.58616200	5.38377800
H	0.58382400	-1.26046200	6.01805500
S	-3.68270000	-1.45064600	5.69770600
H	-3.68427700	-0.26033700	5.07363700
H	-3.55339000	-2.11534500	4.53282700
TS ^{B1-II}			
Si	-3.84640000	5.74340000	-1.76960000
Si	-5.76640000	5.74150000	-0.41200000
Si	-3.84260000	1.90330000	-1.76950000
Si	-5.76260000	1.90120000	-0.41190000
Si	-3.84450000	3.82340000	-3.12730000
Si	-0.00650000	5.74740000	-1.76960000
Si	-1.92640000	5.74530000	-0.41200000
Si	-0.00270000	1.90720000	-1.76950000
Si	-1.92250000	1.90530000	-0.41210000

Si	-0.00440000	3.82730000	-3.12730000
Si	-3.83880000	-1.93680000	-1.76950000
Si	-5.75870000	-1.93870000	-0.41210000
Si	-3.84060000	-0.01670000	-3.12740000
Si	-3.83480000	-5.77680000	-1.76960000
Si	-5.75480000	-5.77890000	-0.41200000
Si	-3.83670000	-3.85680000	-3.12730000
Si	0.00140000	-1.93280000	-1.76950000
Si	-1.91860000	-1.93430000	-0.41190000
Si	-0.00050000	-0.01280000	-3.12730000
Si	0.00530000	-5.77300000	-1.76950000
Si	-1.91490000	-5.77460000	-0.41210000
Si	0.00340000	-3.85290000	-3.12730000
Si	3.83370000	5.75120000	-1.76960000
Si	1.91380000	5.74920000	-0.41210000
Si	3.83750000	1.91110000	-1.76950000
Si	1.91780000	1.90880000	-0.41220000
Si	3.83570000	3.83120000	-3.12730000
Si	5.75380000	5.75300000	-0.41200000
Si	5.75770000	1.91300000	-0.41200000
Si	3.84150000	-1.92910000	-1.76950000
Si	1.92160000	-1.93100000	-0.41230000
Si	3.83960000	-0.00890000	-3.12740000
Si	3.84550000	-5.76910000	-1.76960000
Si	1.92540000	-5.77110000	-0.41210000
Si	3.84350000	-3.84900000	-3.12730000

Si	5.76150000	-1.92660000	-0.41170000
Si	5.76520000	-5.76680000	-0.41200000
H	-3.81700000	6.94060000	-2.68090000
H	-1.90910000	6.93290000	0.50910000
H	-7.08400000	1.93590000	-1.10390000
H	-0.00680000	7.00840000	-2.58130000
H	-7.01330000	5.42270000	-1.17040000
H	-5.89570000	6.99850000	0.38270000
H	-2.98180000	3.85110000	-4.33240000
H	-5.25660000	3.83590000	-3.66500000
H	1.16690000	3.78570000	-4.03000000
H	-1.17770000	3.77770000	-4.02660000
H	-2.98950000	-0.00330000	-4.34430000
H	-5.25530000	-0.00680000	-3.66510000
H	1.16460000	0.00270000	-4.04030000
H	-1.18820000	0.00100000	-4.00970000
H	1.17030000	-3.79370000	-4.03570000
H	-1.17180000	-3.78920000	-4.02370000
H	3.82360000	6.94710000	-2.68240000
H	5.85280000	6.98590000	0.42800000
H	7.02270000	5.47830000	-1.14890000
H	1.90630000	6.94400000	0.49730000
H	7.08790000	1.95490000	-1.08630000
H	5.24900000	3.83760000	-3.66300000
H	2.97340000	3.85830000	-4.33200000
H	7.08850000	-1.90390000	-1.09410000

H	5.24940000	0.00490000	-3.67650000
H	2.97350000	0.00730000	-4.33200000
H	1.91990000	-6.97170000	0.48660000
H	3.83820000	-6.95620000	-2.69450000
H	7.02500000	-5.47450000	-1.15940000
H	5.87500000	-7.00890000	0.40810000
H	5.25620000	-3.83880000	-3.66510000
H	2.98060000	-3.85780000	-4.33210000
H	0.00930000	-7.02340000	-2.59770000
H	-5.86300000	-7.02390000	0.40370000
H	-7.01090000	-5.49010000	-1.16700000
H	-7.07820000	-1.90940000	-1.10900000
H	-3.81630000	-6.96220000	-2.69740000
H	-1.89570000	-6.97200000	0.49120000
H	-2.97450000	-3.86990000	-4.33330000
H	-5.24810000	-3.85970000	-3.66880000
Si	-5.05631000	-0.01675800	0.79839800
Si	-5.05623800	3.83171100	0.83307400
Si	-2.59730400	3.82120500	0.80765400
Si	-5.04958300	-3.86385600	0.81139300
Si	-2.58151100	-0.01114600	0.80659900
Si	-2.59537100	-3.85177200	0.81614200
Si	2.57836600	-0.01301300	0.80570200
Si	2.59156200	3.82801000	0.81653500
Si	5.04388600	3.83445000	0.81399200
Si	2.59696100	-3.84715600	0.80528000

Si	5.05148000	-0.01090400	0.80182300
Si	5.05897700	-3.85669300	0.83085100
S	-5.76736700	-3.67916800	2.85086200
S	-2.15105400	-3.90402400	2.93676600
S	1.79669700	-4.04099300	2.80609800
S	5.78718300	-4.04480400	2.84873700
S	-5.79612100	4.01411900	2.84917300
S	-1.82236000	4.02214000	2.82071700
S	2.10989100	3.91248600	2.92813200
S	5.74272000	3.66453700	2.85998500
S	-5.84747800	0.15054000	2.80440200
S	-2.09487800	0.10574100	2.91032500
S	2.11562500	-0.09117000	2.91002100
S	5.78138500	-0.17821400	2.82798300
H	-5.14320100	-4.77708900	3.31768100
H	-0.81829100	-4.08150700	2.82167600
H	2.11557800	-2.79480600	3.21012500
H	5.19742700	-2.93034400	3.32307300
H	-5.35288600	2.81586100	3.27826300
H	-2.16510700	2.78235800	3.22716200
H	0.82833300	4.29200600	2.75830900
H	5.00260600	4.68572800	3.33125400
H	-5.25240100	-0.95723100	3.28740500
H	5.04832600	0.84175300	3.31588400
Al	0.01198400	-0.03308300	3.60852500
C	0.02993800	1.39681600	5.11194200

H	0.85547500	1.55529300	5.81049000
H	0.18183300	2.16874700	4.33949500
H	-0.92067700	1.61342300	5.60435400
S	0.11289400	-1.69916500	5.29299700
H	-1.22184500	-1.73000000	5.50273900
H	0.12111000	-0.10054600	5.45538400
S	-3.79704000	-1.54523100	5.80828400
H	-3.79948400	-0.32697400	5.24360600
H	-3.51080200	-2.13771900	4.63315700
Im2 ^{B1-II}			
Si	-3.77765600	5.79925700	-1.92284800
Si	-5.69765600	5.79735700	-0.56524800
Si	-3.77385600	1.95915700	-1.92274800
Si	-5.69385600	1.95705700	-0.56514800
Si	-3.77575600	3.87925700	-3.28054800
Si	0.06224400	5.80325700	-1.92284800
Si	-1.85765600	5.80115700	-0.56524800
Si	0.06604400	1.96305700	-1.92274800
Si	-1.85375600	1.96115700	-0.56534800
Si	0.06434400	3.88315700	-3.28054800
Si	-3.77005600	-1.88094300	-1.92274800
Si	-5.68995600	-1.88284300	-0.56534800
Si	-3.77185600	0.03915700	-3.28064800
Si	-3.76605600	-5.72094300	-1.92284800
Si	-5.68605600	-5.72304300	-0.56524800

Si	-3.76795600	-3.80094300	-3.28054800
Si	0.07014400	-1.87694300	-1.92274800
Si	-1.84985600	-1.87844300	-0.56514800
Si	0.06824400	0.04305700	-3.28054800
Si	0.07404400	-5.71714300	-1.92274800
Si	-1.84615600	-5.71874300	-0.56534800
Si	0.07214400	-3.79704300	-3.28054800
Si	3.90244400	5.80705700	-1.92284800
Si	1.98254400	5.80505700	-0.56534800
Si	3.90624400	1.96695700	-1.92274800
Si	1.98654400	1.96465700	-0.56544800
Si	3.90444400	3.88705700	-3.28054800
Si	5.82254400	5.80885700	-0.56524800
Si	5.82644400	1.96885700	-0.56524800
Si	3.91024400	-1.87324300	-1.92274800
Si	1.99034400	-1.87514300	-0.56554800
Si	3.90834400	0.04695700	-3.28064800
Si	3.91424400	-5.71324300	-1.92284800
Si	1.99414400	-5.71524300	-0.56534800
Si	3.91224400	-3.79314300	-3.28054800
Si	5.83024400	-1.87074300	-0.56494800
Si	5.83394400	-5.71094300	-0.56524800
H	-3.74825600	6.99645700	-2.83414800
H	-1.84035600	6.98875700	0.35585200
H	-7.01525600	1.99175700	-1.25714800
H	0.06194400	7.06425700	-2.73454800

H	-6.94455600	5.47855700	-1.32364800
H	-5.82695600	7.05435700	0.22945200
H	-2.91305600	3.90695700	-4.48564800
H	-5.18785600	3.89175700	-3.81824800
H	1.23564400	3.84155700	-4.18324800
H	-1.10895600	3.83355700	-4.17984800
H	-2.92075600	0.05255700	-4.49754800
H	-5.18655600	0.04905700	-3.81834800
H	1.23334400	0.05855700	-4.19354800
H	-1.11945600	0.05685700	-4.16294800
H	1.23904400	-3.73784300	-4.18894800
H	-1.10305600	-3.73334300	-4.17694800
H	3.89234400	7.00295700	-2.83564800
H	5.92154400	7.04175700	0.27475200
H	7.09144400	5.53415700	-1.30214800
H	1.97504400	6.99985700	0.34405200
H	7.15664400	2.01075700	-1.23954800
H	5.31774400	3.89345700	-3.81624800
H	3.04214400	3.91415700	-4.48524800
H	7.15724400	-1.84804300	-1.24734800
H	5.31814400	0.06075700	-3.82974800
H	3.04224400	0.06315700	-4.48524800
H	1.98864400	-6.91584300	0.33335200
H	3.90694400	-6.90034300	-2.84774800
H	7.09374400	-5.41864300	-1.31264800
H	5.94374400	-6.95304300	0.25485200

H	5.32494400	-3.78294300	-3.81834800
H	3.04934400	-3.80194300	-4.48534800
H	0.07804400	-6.96754300	-2.75094800
H	-5.79425600	-6.96804300	0.25045200
H	-6.94215600	-5.43424300	-1.32024800
H	-7.00945600	-1.85354300	-1.26224800
H	-3.74755600	-6.90634300	-2.85064800
H	-1.82695600	-6.91614300	0.33795200
H	-2.90575600	-3.81404300	-4.48654800
H	-5.17935600	-3.80384300	-3.82204800
Si	-4.98998100	0.04179100	0.65054100
Si	-4.98243400	3.88875300	0.68085900
Si	-2.52284800	3.87720100	0.65485700
Si	-4.98219100	-3.80723300	0.65783100
Si	-2.51555000	0.04274300	0.64624800
Si	-2.52759700	-3.79845100	0.66049500
Si	2.63740400	0.04313900	0.64733500
Si	2.66201200	3.88467200	0.66699600
Si	5.11467400	3.89150100	0.65815100
Si	2.67162600	-3.79186700	0.65202000
Si	5.11412500	0.04637900	0.65282200
Si	5.13235400	-3.80065500	0.67793100
S	-5.69513800	-3.61210100	2.69566800
S	-2.07724400	-3.85609800	2.78117900
S	1.87408100	-4.02051100	2.65175800
S	5.86065700	-3.98965200	2.69546700

S	-5.70766000	4.08585300	2.69999200
S	-1.71924900	4.04593200	2.65825000
S	2.22251700	3.94832900	2.78184700
S	5.83605500	3.72005300	2.69655400
S	-5.74853100	0.23480700	2.66290200
S	-1.98577500	0.12290800	2.75775600
S	2.11168000	-0.03513700	2.74909300
S	5.84086600	-0.13790700	2.67719100
H	-5.07078600	-4.70796900	3.16725400
H	-0.76012900	-4.12750200	2.67445000
H	2.29578400	-2.83590100	3.13562300
H	5.27591600	-2.87315000	3.17109800
H	-5.10686700	2.98208700	3.18422400
H	-1.89392100	2.75254000	2.99660400
H	0.90874700	4.22585200	2.65107400
H	5.09687200	4.73555900	3.18087300
H	-5.15687300	-0.87337800	3.14991200
H	5.20066100	0.94585200	3.15894000
Al	0.04760300	-0.50944700	3.32743600
C	-0.10218500	2.25291400	5.24861700
H	-0.23007100	3.30966200	5.48543100
H	0.34944800	2.17801200	4.25557900
H	-1.07672000	1.76111500	5.26938900
S	0.18190200	-1.59142400	5.20498100
H	-1.14871000	-1.66051000	5.41511500
H	0.55607100	1.78569100	5.97984800

S	-3.78718400	-1.55970400	5.65641100
H	-3.64895400	-0.29989800	5.20940600
H	-3.45904500	-2.07562000	4.45814300
Im1 ^{B1-III}			
Si	-3.80450500	5.76722200	-1.93333800
Si	-5.72449000	5.76532000	-0.57573500
Si	-3.80071200	1.92712300	-1.93323600
Si	-5.72068500	1.92504500	-0.57564100
Si	-3.80260400	3.84722600	-3.29103600
Si	0.03539500	5.77122300	-1.93334100
Si	-1.88448700	5.76911400	-0.57573900
Si	0.03919300	1.93100900	-1.93325900
Si	-1.88053700	1.92905200	-0.57587300
Si	0.03749900	3.85112200	-3.29103900
Si	-3.79691400	-1.91299600	-1.93322200
Si	-5.71680500	-1.91485600	-0.57583800
Si	-3.79870200	0.00712200	-3.29114000
Si	-3.79290300	-5.75298000	-1.93333600
Si	-5.71291200	-5.75507900	-0.57573900
Si	-3.79480500	-3.83297900	-3.29103400
Si	0.04327700	-1.90898500	-1.93325800
Si	-1.87678400	-1.91056500	-0.57563300
Si	0.04139400	0.01102400	-3.29104300
Si	0.04719700	-5.74917600	-1.93323800
Si	-1.87301200	-5.75079200	-0.57583700

Si	0.04529700	-3.82907700	-3.29103900
Si	3.87559700	5.77502500	-1.93333700
Si	1.95569600	5.77303300	-0.57583300
Si	3.87940200	1.93493900	-1.93322600
Si	1.95971100	1.93266400	-0.57592100
Si	3.87759600	3.85502200	-3.29103800
Si	5.79569900	5.77682900	-0.57573700
Si	5.79960300	1.93684000	-0.57572700
Si	3.88339800	-1.90526500	-1.93323700
Si	1.96351000	-1.90713500	-0.57603300
Si	3.88149800	0.01492200	-3.29113600
Si	3.88739700	-5.74527600	-1.93333800
Si	1.96729900	-5.74726700	-0.57583800
Si	3.88539700	-3.82517700	-3.29103900
Si	5.80339800	-1.90276300	-0.57543800
Si	5.80709600	-5.74297300	-0.57573800
H	-3.77510500	6.96442400	-2.84463700
H	-1.86719900	6.95672100	0.34536400
H	-7.04210600	1.95973200	-1.26763200
H	0.03509700	7.03222200	-2.74504000
H	-6.97140500	5.44652200	-1.33413400
H	-5.85379900	7.02232300	0.21896200
H	-2.93990300	3.87492300	-4.49613800
H	-5.21470300	3.85972300	-3.82873800
H	1.20879700	3.80952300	-4.19373800
H	-1.13580300	3.80152300	-4.19033800

H	-2.94760300	0.02052300	-4.50803800
H	-5.21340300	0.01702300	-3.82883800
H	1.20649700	0.02652300	-4.20403800
H	-1.14630300	0.02482300	-4.17343800
H	1.21219700	-3.76987700	-4.19943800
H	-1.12990300	-3.76537700	-4.18743800
H	3.86549700	6.97092200	-2.84613900
H	5.89469800	7.00972300	0.26426100
H	7.06459700	5.50212300	-1.31263800
H	1.94819600	6.96782400	0.33356100
H	7.12979600	1.97872300	-1.25004000
H	5.29089700	3.86142300	-3.82673800
H	3.01529700	3.88212300	-4.49573800
H	7.13039700	-1.88007600	-1.25783800
H	5.29129700	0.02872300	-3.84023800
H	3.01539700	0.03112300	-4.49573800
H	1.96179700	-6.94787600	0.32286300
H	3.88009700	-6.93237700	-2.85823700
H	7.06689700	-5.45067700	-1.32313800
H	5.91689600	-6.98507700	0.24436200
H	5.29809700	-3.81497700	-3.82883800
H	3.02249700	-3.83397700	-4.49583800
H	0.05119700	-6.99957700	-2.76143800
H	-5.82110700	-7.00007600	0.23996200
H	-6.96900200	-5.46627700	-1.33074000
H	-7.03630300	-1.88557100	-1.27273900

H	-3.77440200	-6.93837600	-2.86113900
H	-1.85380300	-6.94817800	0.32746100
H	-2.93260300	-3.84607700	-4.49703800
H	-5.20620300	-3.83587700	-3.83253800
Si	-5.00336600	0.00881900	0.63720000
Si	-5.01442600	3.85486600	0.66693300
Si	-2.55799700	3.84475100	0.63995900
Si	-5.00874100	-3.83805200	0.64682000
Si	-2.52337800	0.01471700	0.65660400
Si	-2.55855200	-3.83063500	0.63831600
Si	2.60647100	0.01313500	0.65526800
Si	2.63371700	3.85007800	0.65105800
Si	5.08592800	3.85803200	0.64997700
Si	2.64454600	-3.82239900	0.63793300
Si	5.08355400	0.01238300	0.64017400
Si	5.10630000	-3.83285400	0.66540400
S	-5.69258300	-3.65805000	2.70002600
S	-2.07928900	-3.99606400	2.75760600
S	1.88103700	-4.00554400	2.66036400
S	5.83944900	-4.02574800	2.68092400
S	-5.74490400	4.03330100	2.68677900
S	-1.78828900	4.03230100	2.65354900
S	2.15462200	3.88650000	2.76126400
S	5.78451000	3.68554400	2.69543400
S	-5.79373500	0.17799400	2.64480200
S	-2.01173200	0.07886100	2.74183800

S	2.11307700	-0.11431500	2.74375800
S	5.80689500	-0.15995700	2.66887900
H	-5.07080900	-4.76543200	3.14750600
H	-0.81439100	-4.42607000	2.57902400
H	2.22124900	-2.75252100	3.03157900
H	5.26192800	-2.90496900	3.15522100
H	-5.15008900	2.92015400	3.15747700
H	-2.12396600	2.78820100	3.05390300
H	0.86041600	4.22715400	2.60120200
H	5.04451000	4.70633200	3.16771400
H	-5.19292800	-0.92997200	3.11943700
H	5.04069400	0.83233000	3.16375500
Al	0.08436800	0.41449200	3.55083500
C	0.04141800	1.76283700	4.95454300
H	0.94512000	1.69172000	5.56737600
H	-0.00840400	2.78502500	4.57640700
H	-0.82592900	1.60977500	5.60626900
S	0.07180300	-1.61898900	5.02104600
H	-0.34897500	-2.44866700	4.04232700
H	-1.18510800	-1.47040400	5.51239700
S	-3.68236500	-1.48179400	5.69861000
H	-3.52308400	-2.15428200	4.54283900
H	-3.69061700	-0.29811300	5.06201700
TS ^{B1-III}			
Si	-3.84640000	5.74340000	-1.76960000

Si	-5.76640000	5.74150000	-0.41200000
Si	-3.84260000	1.90330000	-1.76950000
Si	-5.76260000	1.90120000	-0.41190000
Si	-3.84450000	3.82340000	-3.12730000
Si	-0.00650000	5.74740000	-1.76960000
Si	-1.92640000	5.74530000	-0.41200000
Si	-0.00270000	1.90720000	-1.76950000
Si	-1.92250000	1.90530000	-0.41210000
Si	-0.00440000	3.82730000	-3.12730000
Si	-3.83880000	-1.93680000	-1.76950000
Si	-5.75870000	-1.93870000	-0.41210000
Si	-3.84060000	-0.01670000	-3.12740000
Si	-3.83480000	-5.77680000	-1.76960000
Si	-5.75480000	-5.77890000	-0.41200000
Si	-3.83670000	-3.85680000	-3.12730000
Si	0.00140000	-1.93280000	-1.76950000
Si	-1.91860000	-1.93430000	-0.41190000
Si	-0.00050000	-0.01280000	-3.12730000
Si	0.00530000	-5.77300000	-1.76950000
Si	-1.91490000	-5.77460000	-0.41210000
Si	0.00340000	-3.85290000	-3.12730000
Si	3.83370000	5.75120000	-1.76960000
Si	1.91380000	5.74920000	-0.41210000
Si	3.83750000	1.91110000	-1.76950000
Si	1.91780000	1.90880000	-0.41220000
Si	3.83570000	3.83120000	-3.12730000

Si	5.75380000	5.75300000	-0.41200000
Si	5.75770000	1.91300000	-0.41200000
Si	3.84150000	-1.92910000	-1.76950000
Si	1.92160000	-1.93100000	-0.41230000
Si	3.83960000	-0.00890000	-3.12740000
Si	3.84550000	-5.76910000	-1.76960000
Si	1.92540000	-5.77110000	-0.41210000
Si	3.84350000	-3.84900000	-3.12730000
Si	5.76150000	-1.92660000	-0.41170000
Si	5.76520000	-5.76680000	-0.41200000
H	-3.81700000	6.94060000	-2.68090000
H	-1.90910000	6.93290000	0.50910000
H	-7.08400000	1.93590000	-1.10390000
H	-0.00680000	7.00840000	-2.58130000
H	-7.01330000	5.42270000	-1.17040000
H	-5.89570000	6.99850000	0.38270000
H	-2.98180000	3.85110000	-4.33240000
H	-5.25660000	3.83590000	-3.66500000
H	1.16690000	3.78570000	-4.03000000
H	-1.17770000	3.77770000	-4.02660000
H	-2.98950000	-0.00330000	-4.34430000
H	-5.25530000	-0.00680000	-3.66510000
H	1.16460000	0.00270000	-4.04030000
H	-1.18820000	0.00100000	-4.00970000
H	1.17030000	-3.79370000	-4.03570000
H	-1.17180000	-3.78920000	-4.02370000

H	3.82360000	6.94710000	-2.68240000
H	5.85280000	6.98590000	0.42800000
H	7.02270000	5.47830000	-1.14890000
H	1.90630000	6.94400000	0.49730000
H	7.08790000	1.95490000	-1.08630000
H	5.24900000	3.83760000	-3.66300000
H	2.97340000	3.85830000	-4.33200000
H	7.08850000	-1.90390000	-1.09410000
H	5.24940000	0.00490000	-3.67650000
H	2.97350000	0.00730000	-4.33200000
H	1.91990000	-6.97170000	0.48660000
H	3.83820000	-6.95620000	-2.69450000
H	7.02500000	-5.47450000	-1.15940000
H	5.87500000	-7.00890000	0.40810000
H	5.25620000	-3.83880000	-3.66510000
H	2.98060000	-3.85780000	-4.33210000
H	0.00930000	-7.02340000	-2.59770000
H	-5.86300000	-7.02390000	0.40370000
H	-7.01090000	-5.49010000	-1.16700000
H	-7.07820000	-1.90940000	-1.10900000
H	-3.81630000	-6.96220000	-2.69740000
H	-1.89570000	-6.97200000	0.49120000
H	-2.97450000	-3.86990000	-4.33330000
H	-5.24810000	-3.85970000	-3.66880000
Si	-5.04381800	-0.01571300	0.80189100
Si	-5.05291800	3.83176500	0.83057300

Si	-2.59561700	3.81966200	0.80147400
Si	-5.05298600	-3.86325400	0.81104700
Si	-2.56870200	-0.01385000	0.80909500
Si	-2.60112000	-3.85746300	0.80924100
Si	2.56104700	-0.01075100	0.82626700
Si	2.60085500	3.83246400	0.80702800
Si	5.04943600	3.83369600	0.80956100
Si	2.59268200	-3.84678800	0.80865200
Si	5.04157500	-0.01141600	0.80464600
Si	5.05566800	-3.85688400	0.83087500
S	-5.75885700	-3.70100100	2.85783100
S	-2.14667500	-4.03749700	2.92256400
S	1.79023500	-4.03682700	2.80771600
S	5.78121300	-4.04908700	2.84904000
S	-5.77524100	4.01160800	2.85440900
S	-1.80118500	3.94303100	2.81560900
S	2.14487600	3.98122800	2.91938500
S	5.76142700	3.65709600	2.84943600
S	-5.78687600	0.14511700	2.83064900
S	-2.06997200	0.04063800	2.89878300
S	2.09864300	-0.10489300	2.92338200
S	5.78312900	-0.17660000	2.82728400
H	-5.01810700	-4.72177900	3.32881300
H	-0.86591400	-4.42705900	2.75893200
H	2.00871700	-2.75941800	3.18249200
H	5.18493500	-2.93937200	3.32667800

H	-5.17306200	2.90143100	3.32247000
H	-1.99283100	2.63557800	3.09440700
H	0.85727300	4.34294300	2.75359700
H	5.13286500	4.75696500	3.30516900
H	-5.17277900	-0.96834800	3.27796300
H	5.01608800	0.81166500	3.32827400
Al	0.02233300	0.03223100	3.77576100
C	0.11175200	1.71518600	4.96982900
H	0.75082400	2.14892500	4.18277300
H	-0.55503600	2.55517600	5.19166400
H	0.77038000	1.56373900	5.83037100
S	-0.07802600	-1.75522500	5.22761100
H	-0.95173000	-2.42420200	4.44880400
H	-1.48250700	-0.75920700	6.07896800
S	-2.30046900	0.41788000	6.41358000
H	-3.12385600	0.23660600	5.36123700
H	-1.19443900	1.06283600	5.53247200
Im2 ^{B1-III}			
Si	-3.80451700	5.76723700	-1.93332200
Si	-5.72447700	5.76529700	-0.57570000
Si	-3.80069000	1.92711600	-1.93326600
Si	-5.72072100	1.92502000	-0.57573200
Si	-3.80260100	3.84722800	-3.29103900
Si	0.03540100	5.77121700	-1.93337300
Si	-1.88452100	5.76906900	-0.57570000

Si	0.03919200	1.93103300	-1.93321700
Si	-1.88054400	1.92910900	-0.57595400
Si	0.03749800	3.85112900	-3.29103800
Si	-3.79690900	-1.91298900	-1.93322600
Si	-5.71679200	-1.91487400	-0.57577800
Si	-3.79870400	0.00711800	-3.29114400
Si	-3.79290400	-5.75297700	-1.93333800
Si	-5.71289600	-5.75507300	-0.57573400
Si	-3.79480500	-3.83298100	-3.29103400
Si	0.04328200	-1.90896200	-1.93325200
Si	-1.87675700	-1.91039000	-0.57559600
Si	0.04139200	0.01102000	-3.29104800
Si	0.04719600	-5.74917500	-1.93324200
Si	-1.87298800	-5.75077400	-0.57583300
Si	0.04529700	-3.82908300	-3.29102800
Si	3.87560300	5.77502100	-1.93332500
Si	1.95568400	5.77295400	-0.57575300
Si	3.87937500	1.93491000	-1.93329300
Si	1.95968700	1.93265500	-0.57600700
Si	3.87759400	3.85502500	-3.29105000
Si	5.79568500	5.77682000	-0.57569700
Si	5.79962300	1.93681400	-0.57581200
Si	3.88341500	-1.90528600	-1.93319900
Si	1.96352500	-1.90712200	-0.57606400
Si	3.88149600	0.01491800	-3.29114400
Si	3.88739800	-5.74527500	-1.93333500

Si	1.96729000	-5.74726600	-0.57581100
Si	3.88539700	-3.82518000	-3.29103100
Si	5.80337700	-1.90278000	-0.57540600
Si	5.80709400	-5.74297100	-0.57572700
H	-3.77510700	6.96442900	-2.84463000
H	-1.86717100	6.95671300	0.34537400
H	-7.04210000	1.95972700	-1.26764300
H	0.03509800	7.03222000	-2.74504200
H	-6.97140700	5.44652400	-1.33413200
H	-5.85380100	7.02232200	0.21896400
H	-2.93990300	3.87492300	-4.49613800
H	-5.21470300	3.85972300	-3.82873800
H	1.20879700	3.80952300	-4.19373800
H	-1.13580300	3.80152300	-4.19033800
H	-2.94760300	0.02052300	-4.50803800
H	-5.21340300	0.01702300	-3.82883800
H	1.20649700	0.02652300	-4.20403800
H	-1.14630300	0.02482300	-4.17343800
H	1.21219700	-3.76987700	-4.19943800
H	-1.12990300	-3.76537700	-4.18743800
H	3.86550100	6.97093300	-2.84612500
H	5.89468900	7.00971800	0.26427000
H	7.06459900	5.50212500	-1.31263500
H	1.94818600	6.96781500	0.33357300
H	7.12978400	1.97872600	-1.25006300
H	5.29089700	3.86142300	-3.82673800

H	3.01529700	3.88212300	-4.49573800
H	7.13040700	-1.88007900	-1.25781900
H	5.29129700	0.02872300	-3.84023800
H	3.01539700	0.03112300	-4.49573800
H	1.96179700	-6.94787700	0.32286200
H	3.88009700	-6.93237500	-2.85824000
H	7.06689600	-5.45067600	-1.32313900
H	5.91689800	-6.98507700	0.24436100
H	5.29809700	-3.81497700	-3.82883800
H	3.02249700	-3.83397700	-4.49583800
H	0.05119800	-6.99957600	-2.76144000
H	-5.82110200	-7.00007700	0.23996200
H	-6.96900300	-5.46627600	-1.33073700
H	-7.03630300	-1.88558000	-1.27273900
H	-3.77440400	-6.93837800	-2.86113700
H	-1.85380200	-6.94817700	0.32746200
H	-2.93260300	-3.84607700	-4.49703800
H	-5.20620300	-3.83587700	-3.83253800
Si	-5.01526200	0.00838900	0.63494700
Si	-5.00955600	3.85551300	0.67698200
Si	-2.55029700	3.84703400	0.64412200
Si	-5.00679800	-3.83943700	0.65013100
Si	-2.54331500	0.01369400	0.63074600
Si	-2.55091600	-3.82826500	0.65188100
Si	2.60818600	0.01015600	0.64055100
Si	2.63618800	3.85183700	0.65727400

Si	5.08885400	3.86000300	0.64709300
Si	2.64613500	-3.82467200	0.64233300
Si	5.08617600	0.01435100	0.64387800
Si	5.10612100	-3.83252300	0.66644200
S	-5.70867000	-3.67569400	2.69724200
S	-2.06649100	-3.87204000	2.76482100
S	1.86014700	-4.06698700	2.64423300
S	5.83737100	-4.01984500	2.68337300
S	-5.71985500	4.04507200	2.70095200
S	-1.74440800	4.08392900	2.63593300
S	2.21003800	3.89073200	2.77307900
S	5.81739100	3.69191100	2.68381700
S	-5.75548700	0.17290500	2.65625400
S	-2.02293800	0.11600400	2.73775300
S	2.08008500	-0.09144100	2.74419600
S	5.81245800	-0.16667300	2.66914500
H	-4.95431900	-4.68504600	3.17149500
H	-0.77567700	-4.23167500	2.61775700
H	2.25556700	-2.87247700	3.12466600
H	5.25151000	-2.90397200	3.15909100
H	-5.07989300	2.97046200	3.20654500
H	-2.09106000	2.86643000	3.09703900
H	0.88178700	4.09611900	2.65737100
H	5.08288400	4.71070000	3.16807600
H	-5.13758000	-0.93724700	3.10783200
H	5.17092600	0.91759600	3.14818700

Al	0.00271800	-0.51689100	3.31402800
C	0.35110900	2.21980100	5.20907100
H	-0.05768300	2.14082200	4.19733500
H	0.31337400	3.27041900	5.50076800
H	1.38738200	1.88115400	5.20713900
S	0.01926400	-1.61995700	5.19204000
H	-1.31217300	-1.81682900	5.16966800
H	-4.10462900	1.96767400	6.51700900
S	-3.41189900	1.80332400	5.37868300
H	-3.85619700	0.55348800	5.18584500
H	-0.24682200	1.62798600	5.90054100
P^{B1}			
Si	23.54399900	13.33659800	-2.71529800
Si	21.62400400	13.33468300	-1.35769300
Si	23.54778300	9.49647800	-2.71517600
Si	21.62785200	9.49433900	-1.35763900
Si	23.54590100	11.41659800	-4.07300500
Si	27.38389900	13.34059700	-2.71530200
Si	25.46399800	13.33847600	-1.35769700
Si	27.38770500	9.50035700	-2.71526200
Si	25.46777000	9.49839000	-1.35775900
Si	27.38599900	11.42049700	-4.07300600
Si	23.55157900	5.65640200	-2.71516200
Si	21.63176900	5.65452600	-1.35781200
Si	23.54980000	7.57649900	-4.07309300

Si	23.55559900	1.81640500	-2.71530000
Si	21.63561000	1.81431800	-1.35770000
Si	23.55370100	3.73640100	-4.07300400
Si	27.39179200	5.66044900	-2.71525600
Si	25.47165600	5.65902100	-1.35759400
Si	27.38989800	7.58039700	-4.07299900
Si	27.39569800	1.82020300	-2.71520200
Si	25.47549900	1.81864600	-1.35779400
Si	27.39380400	3.74029800	-4.07299900
Si	31.22410100	13.34440000	-2.71529800
Si	29.30419400	13.34238200	-1.35779900
Si	31.22791600	9.50431000	-2.71517400
Si	29.30829600	9.50196900	-1.35789200
Si	31.22610100	11.42440000	-4.07300200
Si	33.14420000	13.34619400	-1.35769700
Si	33.14807400	9.50619500	-1.35769800
Si	31.23190700	5.66409900	-2.71518900
Si	29.31206600	5.66228300	-1.35804300
Si	31.22999700	7.58430000	-4.07310000
Si	31.23589900	1.82410200	-2.71530000
Si	29.31579700	1.82211400	-1.35779300
Si	31.23390100	3.74420100	-4.07300200
Si	33.15187100	5.66661900	-1.35742000
Si	33.15560100	1.82640500	-1.35769700
H	23.57339900	14.53380200	-3.62659800
H	25.48130500	14.52609700	-0.43659700

H	20.30640600	9.52908900	-2.04961100
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01589800	-2.11609900
H	21.49469800	14.59169800	-0.56299700
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030100	-3.62809900
H	33.24320100	14.57909900	-0.51769900
H	34.41310000	13.07150000	-2.09460000
H	29.29669700	14.53719800	-0.44839800
H	34.47829600	9.54809400	-2.03200800
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889800	5.68930400	-2.03980300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31029800	0.62150200	-0.45909800
H	31.22860000	0.63699900	-3.64019900

H	34.41540000	2.11870000	-2.10510000
H	33.26540100	0.58430100	-0.53759900
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56979900	-3.54339900
H	21.52740000	0.56930100	-0.54199800
H	20.37949900	2.10310200	-2.11269800
H	20.31220200	5.68380900	-2.05470300
H	23.57409900	0.63099800	-3.64309800
H	25.49470800	0.62120400	-0.45449500
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.34591600	7.57580000	-0.13861800
Si	22.32888800	11.42469300	-0.11363500
Si	24.78589800	11.41549900	-0.14032000
Si	22.33996200	3.72926300	-0.13405900
Si	24.82365100	7.58267600	-0.14508400
Si	24.79617300	3.74009400	-0.12432400
Si	29.97045200	7.58168700	-0.14661800
Si	29.97897900	11.42074100	-0.12936700
Si	32.43256500	11.42738500	-0.13087800
Si	29.98597700	3.74599600	-0.13789100
Si	32.44253800	7.58104300	-0.14180500
Si	32.44832200	3.73542200	-0.11441300
S	21.61369900	3.90375500	1.90208000
S	25.23653300	3.68596500	1.98934100

S	29.18838600	3.55968000	1.86608900
S	33.17812900	3.53483800	1.90158700
S	21.59355500	11.61211500	1.90289800
S	25.56171700	11.63818700	1.87040200
S	29.47412400	11.45616100	1.97953800
S	33.12614400	11.24780700	1.91547300
S	21.62101300	7.76216400	1.88770700
S	25.37108400	7.68458200	1.95522700
S	29.45454100	7.49776000	1.96396400
S	33.16133700	7.39009800	1.88390900
H	22.35728200	2.89265200	2.38907900
H	26.55838800	3.45079100	1.85474500
H	29.37752800	4.84670400	2.21896200
H	32.58272300	4.64009000	2.38948400
H	22.17343800	10.49266000	2.37688300
H	25.13644500	10.44505000	2.33026600
H	28.21467100	11.90703400	1.82046400
H	32.36527100	12.24812900	2.39862400
H	22.25908700	6.67569200	2.36623700
H	32.51381000	8.46847000	2.36738900
Al	27.44177900	8.16881900	2.51120900
S	27.48066900	9.13506200	4.46094900
H	26.15002000	9.04306000	4.63708800

P^{Al}

Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400

Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000

H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31246800	7.57639600	-0.13986500

Si	22.32574100	11.42534500	-0.11265100
Si	24.77905200	11.41528100	-0.14019600
Si	22.33257500	3.72898100	-0.13554100
Si	24.77454000	7.57612200	-0.18494500
Si	24.78346100	3.74037100	-0.13835900
Si	29.97163500	7.58249200	-0.09747800
Si	29.99007500	11.42394000	-0.13372200
Si	32.43944400	11.42628700	-0.13690300
Si	29.97901400	3.74733400	-0.14184400
Si	32.44790100	7.58263400	-0.14988500
Si	32.44360700	3.73722900	-0.11413500
S	21.62118700	3.91144800	1.90673500
S	25.21881500	3.72191100	1.98627200
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S	33.15783800	3.54801200	1.90735900
S	21.58462400	11.61750100	1.90134000
S	25.55126200	11.63034300	1.86757600
S	29.55708200	11.51463100	1.97891800
S	33.16029500	11.24891600	1.89848800
S	21.58300000	7.76674000	1.88399500
S	25.46396600	7.61911500	1.92090800
S	29.65104400	7.45592700	2.00489700
S	33.24539100	7.42046000	1.85019200
H	22.34650900	2.88657400	2.39179800
H	26.55103100	3.53059500	1.86232500
H	29.39013800	4.86153100	2.20657000

H	32.57133600	4.66856300	2.37234100
H	22.17322200	10.50836900	2.38771300
H	25.18208300	10.42483400	2.34203500
H	28.25741600	11.83763200	1.83530300
H	32.52874600	12.34512600	2.35889900
H	22.17791000	6.65521700	2.35904600
H	25.23642500	6.31290500	2.19451400
H	32.45618500	8.37302400	2.38494100
Al	27.72273400	7.72646800	3.17874600
C	27.35469600	6.05510000	4.13539300
C	27.47522100	9.44432500	4.06381100
H	26.43799100	6.11434100	4.73103500
H	27.26304500	5.19287500	3.47127900
H	28.17404000	5.83716600	4.82914800
H	28.31458300	9.61439600	4.74644600
H	27.44244600	10.29930800	3.39178000
H	26.55905200	9.43868000	4.66375400
Im1 ^{B2-up}			
Si	-3.89947700	5.73982400	-1.89328400
Si	-5.81947700	5.73792400	-0.53568400
Si	-3.89567700	1.89972400	-1.89318400
Si	-5.81567700	1.89762400	-0.53558400
Si	-3.89757700	3.81982400	-3.25098400
Si	-0.05957700	5.74382400	-1.89328400
Si	-1.97947700	5.74172400	-0.53568400

Si	-0.05577700	1.90362400	-1.89318400
Si	-1.97557700	1.90172400	-0.53578400
Si	-0.05747700	3.82372400	-3.25098400
Si	-3.89187700	-1.94037600	-1.89318400
Si	-5.81177700	-1.94227600	-0.53578400
Si	-3.89367700	-0.02027600	-3.25108400
Si	-3.88787700	-5.78037600	-1.89328400
Si	-5.80787700	-5.78247600	-0.53568400
Si	-3.88977700	-3.86037600	-3.25098400
Si	-0.05167700	-1.93637600	-1.89318400
Si	-1.97167700	-1.93787600	-0.53558400
Si	-0.05357700	-0.01637600	-3.25098400
Si	-0.04777700	-5.77657600	-1.89318400
Si	-1.96797700	-5.77817600	-0.53578400
Si	-0.04967700	-3.85647600	-3.25098400
Si	3.78062300	5.74762400	-1.89328400
Si	1.86072300	5.74562400	-0.53578400
Si	3.78442300	1.90752400	-1.89318400
Si	1.86472300	1.90522400	-0.53588400
Si	3.78262300	3.82762400	-3.25098400
Si	5.70072300	5.74942400	-0.53568400
Si	5.70462300	1.90942400	-0.53568400
Si	3.78842300	-1.93267600	-1.89318400
Si	1.86852300	-1.93457600	-0.53598400
Si	3.78652300	-0.01247600	-3.25108400
Si	3.79242300	-5.77267600	-1.89328400

Si	1.87232300	-5.77467600	-0.53578400
Si	3.79042300	-3.85257600	-3.25098400
Si	5.70842300	-1.93017600	-0.53538400
Si	5.71212300	-5.77037600	-0.53568400
H	-3.87007700	6.93702400	-2.80458400
H	-1.96217700	6.92932400	0.38541600
H	-7.13707700	1.93232400	-1.22758400
H	-0.05987700	7.00482400	-2.70498400
H	-7.06637700	5.41912400	-1.29408400
H	-5.94877700	6.99492400	0.25901600
H	-3.03487700	3.84752400	-4.45608400
H	-5.30967700	3.83232400	-3.78868400
H	1.11382300	3.78212400	-4.15368400
H	-1.23077700	3.77412400	-4.15028400
H	-3.04257700	-0.00687600	-4.46798400
H	-5.30837700	-0.01037600	-3.78878400
H	1.11152300	-0.00087600	-4.16398400
H	-1.24127700	-0.00257600	-4.13338400
H	1.11722300	-3.79727600	-4.15938400
H	-1.22487700	-3.79277600	-4.14738400
H	3.77052300	6.94352400	-2.80608400
H	5.79972300	6.98232400	0.30431600
H	6.96962300	5.47472400	-1.27258400
H	1.85322300	6.94042400	0.37361600
H	7.03482300	1.95132400	-1.20998400
H	5.19592300	3.83402400	-3.78668400

H	2.92032300	3.85472400	-4.45568400
H	7.03542300	-1.90747600	-1.21778400
H	5.19632300	0.00132400	-3.80018400
H	2.92042300	0.00372400	-4.45568400
H	1.86682300	-6.97527600	0.36291600
H	3.78512300	-6.95977600	-2.81818400
H	6.97192300	-5.47807600	-1.28308400
H	5.82192300	-7.01247600	0.28441600
H	5.20312300	-3.84237600	-3.78878400
H	2.92752300	-3.86137600	-4.45578400
H	-0.04377700	-7.02697600	-2.72138400
H	-5.91607700	-7.02747600	0.28001600
H	-7.06397700	-5.49367600	-1.29068400
H	-7.13127700	-1.91297600	-1.23268400
H	-3.86937700	-6.96577600	-2.82108400
H	-1.94877700	-6.97557600	0.36751600
H	-3.02757700	-3.87347600	-4.45698400
H	-5.30117700	-3.86327600	-3.79248400
Si	-5.11944700	-0.02088400	0.67794900
Si	-5.11945400	3.82738000	0.70524300
Si	-2.66712100	3.82211000	0.67623800
Si	-5.10918100	-3.86738000	0.68499700
Si	-2.65940100	-0.02152300	0.65692200
Si	-2.65725500	-3.85534800	0.68519900
Si	2.55614900	-0.01705200	0.72468900
Si	2.54438500	3.82447400	0.69045800

Si	4.99338400	3.82921000	0.68654700
Si	2.53323300	-3.84992000	0.68128000
Si	5.03083200	-0.01395100	0.66097100
Si	4.99714400	-3.85796200	0.70885600
S	-5.82752300	-3.69345400	2.72610300
S	-2.23239600	-3.88758300	2.81027600
S	1.70526900	-4.02985500	2.67295500
S	5.70905400	-4.02125300	2.73481600
S	-5.86602600	4.01518400	2.71840800
S	-1.92314800	4.08724100	2.68637000
S	2.11544000	3.89583800	2.81179400
S	5.70900300	3.67265800	2.73222400
S	-5.85612000	0.16331400	2.70243800
S	-1.89144500	0.09479800	2.69054500
S	2.38928800	-0.17725700	2.84395400
S	5.91930500	-0.14871400	2.62830100
H	-5.10283800	-4.72025400	3.20809300
H	-0.90033500	-4.07762600	2.69153600
H	1.96177800	-2.75704400	3.04465800
H	5.12015200	-2.89351100	3.17977200
H	-5.28619700	2.89910700	3.19967200
H	-2.30443400	2.88924000	3.17064800
H	0.80331900	4.18012800	2.69215200
H	5.08213000	4.77911500	3.17415300
H	-5.24927300	-0.94173500	3.17747500
H	-2.24673600	-1.15237900	3.06670300

H	5.17870800	0.84498300	3.15474600
Al	0.73499100	0.12368200	4.37738500
C	0.03390800	-1.58894900	5.01699500
C	0.00411700	1.88400300	4.80201800
H	-0.81269900	-1.45859000	5.69888500
H	-0.31579600	-2.19897100	4.18004800
H	0.79237800	-2.17774800	5.54231500
H	0.66035400	2.51126100	5.41063400
H	-0.18585400	2.42942500	3.87946600
H	-0.95086300	1.77898700	5.32828900
S	2.86294300	0.33016200	5.99634100
H	2.32732800	0.97629000	7.04690600
H	3.24212400	1.46781400	5.38685900
TS ^{B2-up}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000

Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50200000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000

H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
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H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
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H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000

H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32234300	7.57596800	-0.14535800
Si	22.32527300	11.42453400	-0.11496600
Si	24.77925600	11.41600000	-0.14319100
Si	22.33294000	3.72940600	-0.13733300
Si	24.77900700	7.57518800	-0.17251300
Si	24.78411400	3.74121500	-0.13841800
Si	30.00753000	7.58066100	-0.09668600
Si	29.98954500	11.42343000	-0.13481800
Si	32.43880200	11.42529800	-0.13252600
Si	29.98186100	3.74729900	-0.14177100
Si	32.48415500	7.58520100	-0.15882000
Si	32.44662800	3.73789100	-0.11045900

S	21.61493300	3.90402900	1.90368300
S	25.20532500	3.70322800	1.98778500
S	29.15315000	3.57346800	1.85237800
S	33.16813700	3.56580800	1.90995200
S	21.58103100	11.61398800	1.89890100
S	25.53478600	11.63878300	1.87301300
S	29.53401900	11.51872900	1.98017100
S	33.14670600	11.24191700	1.90737200
S	21.59424100	7.76081100	1.88228400
S	25.56492500	7.68251900	1.84957400
S	29.92522500	7.48391800	2.04471600
S	33.40447900	7.43501800	1.79069100
H	22.33335500	2.87243800	2.38466000
H	26.53712400	3.51359700	1.87027900
H	29.49343300	4.81736600	2.25057000
H	32.76331400	4.78912500	2.30804100
H	22.16143100	10.49808200	2.37973300
H	25.14885700	10.43054400	2.32870300
H	28.23695000	11.85060700	1.82697900
H	32.51364400	12.33750300	2.36723600
H	22.20195500	6.65500400	2.35449000
H	25.22016800	6.43266200	2.22510100
H	32.62817000	8.35480200	2.39506800
Al	28.34816600	7.59755200	3.61583500
C	27.33232500	6.03972800	4.19061900
C	27.50596200	9.47232400	3.93963900

H	26.40461900	6.30595200	4.70622900
H	27.06923500	5.40666200	3.34087600
H	27.93179900	5.43102100	4.87422400
H	27.86386800	10.40870900	4.38241300
H	27.39170700	9.70746000	2.87797500
H	26.53004500	9.25123400	4.38100900
S	29.93227200	8.18163000	5.35972600
H	29.13480200	7.73918700	6.34913600
H	28.72728900	9.05103000	4.72668800
Im2 ^{B2-up}			
Si	-3.89946400	5.73980300	-1.89329400
Si	-5.81946300	5.73793700	-0.53573100
Si	-3.89568600	1.89969700	-1.89314800
Si	-5.81564000	1.89764000	-0.53550400
Si	-3.89757600	3.81982000	-3.25098100
Si	-0.05955800	5.74381800	-1.89325300
Si	-1.97940000	5.74173800	-0.53573000
Si	-0.05568400	1.90365900	-1.89327600
Si	-1.97561200	1.90175900	-0.53569500
Si	-0.05748200	3.82372800	-3.25098100
Si	-3.89187300	-1.94037100	-1.89318300
Si	-5.81178300	-1.94227500	-0.53577600
Si	-3.89367800	-0.02027400	-3.25108200
Si	-3.88787700	-5.78037600	-1.89328300
Si	-5.80787400	-5.78247300	-0.53568300

Si	-3.88977700	-3.86037500	-3.25098600
Si	-0.05166000	-1.93638900	-1.89319600
Si	-1.97168300	-1.93788900	-0.53556100
Si	-0.05357500	-0.01637800	-3.25099800
Si	-0.04777900	-5.77658100	-1.89317900
Si	-1.96798000	-5.77817100	-0.53579000
Si	-0.04967800	-3.85647300	-3.25099000
Si	3.78062300	5.74762500	-1.89328000
Si	1.86071500	5.74568900	-0.53584200
Si	3.78444000	1.90759900	-1.89322100
Si	1.86452700	1.90501400	-0.53577400
Si	3.78263300	3.82763700	-3.25096800
Si	5.70071600	5.74942300	-0.53570000
Si	5.70459100	1.90946800	-0.53557700
Si	3.78843500	-1.93267100	-1.89316700
Si	1.86857400	-1.93462000	-0.53610200
Si	3.78651700	-0.01248800	-3.25109100
Si	3.79242600	-5.77268200	-1.89328200
Si	1.87234000	-5.77469400	-0.53580800
Si	3.79043000	-3.85258500	-3.25096900
Si	5.70838600	-1.93013800	-0.53545400
Si	5.71211000	-5.77036600	-0.53566400
H	-3.87007600	6.93701300	-2.80459800
H	-1.96218200	6.92933100	0.38540800
H	-7.13707600	1.93233600	-1.22758500
H	-0.05988400	7.00482300	-2.70498600

H	-7.06638000	5.41912200	-1.29407900
H	-5.94877800	6.99492800	0.25901000
H	-3.03487700	3.84752400	-4.45608400
H	-5.30967700	3.83232400	-3.78868400
H	1.11382300	3.78212400	-4.15368400
H	-1.23077700	3.77412400	-4.15028400
H	-3.04257700	-0.00687600	-4.46798400
H	-5.30837700	-0.01037600	-3.78878400
H	1.11152300	-0.00087600	-4.16398400
H	-1.24127700	-0.00257600	-4.13338400
H	1.11722300	-3.79727600	-4.15938400
H	-1.22487700	-3.79277600	-4.14738400
H	3.77052500	6.94352700	-2.80608100
H	5.79972200	6.98231900	0.30432300
H	6.96962800	5.47472300	-1.27257600
H	1.85321300	6.94041800	0.37362400
H	7.03480500	1.95131700	-1.21002000
H	5.19592300	3.83402400	-3.78668400
H	2.92032300	3.85472400	-4.45568400
H	7.03543800	-1.90747900	-1.21775500
H	5.19632300	0.00132400	-3.80018400
H	2.92042300	0.00372400	-4.45568400
H	1.86680800	-6.97527400	0.36291800
H	3.78512400	-6.95977400	-2.81818600
H	6.97192300	-5.47807300	-1.28308300
H	5.82192900	-7.01247700	0.28441400

H	5.20312300	-3.84237600	-3.78878400
H	2.92752300	-3.86137600	-4.45578400
H	-0.04377700	-7.02697500	-2.72138600
H	-5.91607500	-7.02747500	0.28001700
H	-7.06397800	-5.49367400	-1.29068200
H	-7.13127600	-1.91297100	-1.23268600
H	-3.86937800	-6.96577600	-2.82108400
H	-1.94877500	-6.97557600	0.36751600
H	-3.02757700	-3.87347600	-4.45698400
H	-5.30117700	-3.86327600	-3.79248400
Si	-5.13006700	-0.01994100	0.68344600
Si	-5.10985800	3.82875500	0.71183200
Si	-2.65661800	3.82146400	0.68247200
Si	-5.11166100	-3.86775800	0.68681100
Si	-2.66783000	-0.02069900	0.62895000
Si	-2.66077100	-3.85594200	0.68299100
Si	2.53067100	-0.01483400	0.71667400
Si	2.53910700	3.82499900	0.69688600
Si	4.99277500	3.83072700	0.68856100
Si	2.53787600	-3.84967500	0.68036800
Si	5.00742900	-0.01233100	0.67190200
Si	5.00350500	-3.85981000	0.70941400
S	-5.82021600	-3.68570400	2.72999200
S	-2.22171000	-3.87297100	2.80898300
S	1.71388000	-4.03334000	2.67454400
S	5.72988000	-4.04710800	2.72667700

S	-5.82815600	4.01570900	2.73483200
S	-1.83979600	4.05636000	2.66309900
S	2.11794600	3.85742700	2.81093600
S	5.71396600	3.65845000	2.72465800
S	-5.84173800	0.17010700	2.71309800
S	-1.95310500	-0.00618100	2.73088700
S	2.22310900	-0.14332000	2.83191300
S	5.81107300	-0.16934900	2.67058000
H	-5.09789100	-4.71372400	3.21288500
H	-0.88968300	-4.06300500	2.68276500
H	2.01948900	-2.77751600	3.06655600
H	5.30717600	-2.83715900	3.14581500
H	-5.21842400	2.91526900	3.21694300
H	-2.16703200	2.85048200	3.16131700
H	0.79340900	4.08855400	2.70873200
H	4.98385100	4.68227100	3.20517100
H	-5.24536500	-0.94352000	3.18215700
H	-2.17527800	-1.31780300	2.98734000
H	5.02841800	0.78583900	3.21041100
Al	0.29827900	0.09137100	3.95809800
C	-0.14946500	-1.49418900	5.00542400
C	-3.85911500	2.12479400	5.52380100
H	-1.09993300	-1.38875500	5.53824900
H	-0.21127300	-2.39545700	4.39041200
H	0.62712600	-1.66467300	5.75776400
H	-4.94229600	2.15700000	5.64485800

H	-3.47601700	3.13622600	5.38432200
H	-3.61147900	1.50861500	4.65745800
S	0.11588700	2.05869300	4.95327100
H	-0.86282100	1.60573900	5.76105700
H	-3.41408700	1.68769600	6.41792600
p^{B2-up}			
Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400

Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000

H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000

H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31303900	7.57670600	-0.13859500
Si	22.33160800	11.42576800	-0.11137000
Si	24.78600700	11.41817500	-0.13761000
Si	22.33193500	3.72886000	-0.13534600
Si	24.77618800	7.57645300	-0.19004700
Si	24.78281100	3.74082300	-0.13925100
Si	29.97568500	7.58197400	-0.10746400
Si	29.98326500	11.42171700	-0.12544000
Si	32.43677200	11.42750900	-0.13383700
Si	29.98077100	3.74712200	-0.14212700
Si	32.45237600	7.58315800	-0.14862400
Si	32.44562200	3.73727800	-0.11353300
S	21.62319100	3.90942200	1.90799300
S	25.22231900	3.72424900	1.98651400
S	29.15937700	3.56894800	1.85405000
S	33.16144600	3.54867400	1.90745900
S	21.59410000	11.61572700	1.90437200
S	25.59710800	11.65540200	1.84582600
S	29.56250900	11.45279400	1.98860300
S	33.15826200	11.25525200	1.90209300

S	21.59031100	7.76388900	1.88771700
S	25.48523400	7.60277100	1.91542600
S	29.66561500	7.45027600	2.00703500
S	33.24516300	7.41824700	1.85227000
H	22.34710800	2.88250500	2.39089500
H	26.55382900	3.53055100	1.86003200
H	29.44205200	4.83447600	2.23249700
H	32.58016900	4.67223000	2.37171300
H	22.19138900	10.51109600	2.39053000
H	25.26785200	10.45017000	2.34390300
H	28.23794900	11.68336600	1.88706600
H	32.42737200	12.27818700	2.38329600
H	22.18221400	6.64842700	2.35728600
H	25.25949900	6.29294900	2.17650400
H	32.47624000	8.39212500	2.37881200
Al	27.74403100	7.68560600	3.13713300
C	27.30054500	6.09531900	4.17930400
H	26.35535600	6.19670400	4.72155600
H	27.23330400	5.19741300	3.56004700
H	28.08405700	5.92041700	4.92349300
S	27.58615200	9.65070800	4.13920900
H	26.61645500	9.20476400	4.96168800
Im1 ^{B2-down}			
Si	-3.91511900	5.73622800	-1.89118600
Si	-5.83511900	5.73432800	-0.53358600

Si	-3.91131900	1.89612800	-1.89108600
Si	-5.83131900	1.89402800	-0.53348600
Si	-3.91321900	3.81622800	-3.24888600
Si	-0.07521900	5.74022800	-1.89118600
Si	-1.99511900	5.73812800	-0.53358600
Si	-0.07141900	1.90002800	-1.89108600
Si	-1.99121900	1.89812800	-0.53368600
Si	-0.07311900	3.82012800	-3.24888600
Si	-3.90751900	-1.94397200	-1.89108600
Si	-5.82741900	-1.94587200	-0.53368600
Si	-3.90931900	-0.02387200	-3.24898600
Si	-3.90351900	-5.78397200	-1.89118600
Si	-5.82351900	-5.78607200	-0.53358600
Si	-3.90541900	-3.86397200	-3.24888600
Si	-0.06731900	-1.93997200	-1.89108600
Si	-1.98731900	-1.94147200	-0.53348600
Si	-0.06921900	-0.01997200	-3.24888600
Si	-0.06341900	-5.78017200	-1.89108600
Si	-1.98361900	-5.78177200	-0.53368600
Si	-0.06531900	-3.86007200	-3.24888600
Si	3.76498100	5.74402800	-1.89118600
Si	1.84508100	5.74202800	-0.53368600
Si	3.76878100	1.90392800	-1.89108600
Si	1.84908100	1.90162800	-0.53378600
Si	3.76698100	3.82402800	-3.24888600
Si	5.68508100	5.74582800	-0.53358600

Si	5.68898100	1.90582800	-0.53358600
Si	3.77278100	-1.93627200	-1.89108600
Si	1.85288100	-1.93817200	-0.53388600
Si	3.77088100	-0.01607200	-3.24898600
Si	3.77678100	-5.77627200	-1.89118600
Si	1.85668100	-5.77827200	-0.53368600
Si	3.77478100	-3.85617200	-3.24888600
Si	5.69278100	-1.93377200	-0.53328600
Si	5.69648100	-5.77397200	-0.53358600
H	-3.88571900	6.93342800	-2.80248600
H	-1.97781900	6.92572800	0.38751400
H	-7.15271900	1.92872800	-1.22548600
H	-0.07551900	7.00122800	-2.70288600
H	-7.08201900	5.41552800	-1.29198600
H	-5.96441900	6.99132800	0.26111400
H	-3.05051900	3.84392800	-4.45398600
H	-5.32531900	3.82872800	-3.78658600
H	1.09818100	3.77852800	-4.15158600
H	-1.24641900	3.77052800	-4.14818600
H	-3.05821900	-0.01047200	-4.46588600
H	-5.32401900	-0.01397200	-3.78668600
H	1.09588100	-0.00447200	-4.16188600
H	-1.25691900	-0.00617200	-4.13128600
H	1.10158100	-3.80087200	-4.15728600
H	-1.24051900	-3.79637200	-4.14528600
H	3.75488100	6.93992800	-2.80398600

H	5.78408100	6.97872800	0.30641400
H	6.95398100	5.47112800	-1.27048600
H	1.83758100	6.93682800	0.37571400
H	7.01918100	1.94772800	-1.20788600
H	5.18028100	3.83042800	-3.78458600
H	2.90468100	3.85112800	-4.45358600
H	7.01978100	-1.91107200	-1.21568600
H	5.18068100	-0.00227200	-3.79808600
H	2.90478100	0.00012800	-4.45358600
H	1.85118100	-6.97887200	0.36501400
H	3.76948100	-6.96337200	-2.81608600
H	6.95628100	-5.48167200	-1.28098600
H	5.80628100	-7.01607200	0.28651400
H	5.18748100	-3.84597200	-3.78668600
H	2.91188100	-3.86497200	-4.45368600
H	-0.05941900	-7.03057200	-2.71928600
H	-5.93171900	-7.03107200	0.28211400
H	-7.07961900	-5.49727200	-1.28858600
H	-7.14691900	-1.91657200	-1.23058600
H	-3.88501900	-6.96937200	-2.81898600
H	-1.96441900	-6.97917200	0.36961400
H	-3.04321900	-3.87707200	-4.45488600
H	-5.31681900	-3.86687200	-3.79038600
Si	-5.13519100	-0.02449400	0.67997000
Si	-5.13484900	3.82379200	0.70749200
Si	-2.68237300	3.81830400	0.67870500

Si	-5.12520800	-3.87098600	0.68686800
Si	-2.67532100	-0.02474800	0.65863900
Si	-2.67346400	-3.85898800	0.68714500
Si	2.54037400	-0.02088000	0.72839500
Si	2.52840500	3.82107200	0.69270900
Si	4.97752100	3.82547600	0.68894200
Si	2.51852800	-3.85355800	0.68330000
Si	5.01463100	-0.01629900	0.66086000
Si	4.98310900	-3.86198200	0.71221200
S	-5.84457200	-3.69715500	2.72760600
S	-2.25109400	-3.89088300	2.81230300
S	1.68750600	-4.03772600	2.67264700
S	5.70269900	-4.01886500	2.73631800
S	-5.88128300	4.01156100	2.72070100
S	-1.93725600	4.08237800	2.68875500
S	2.09976700	3.89237000	2.81342800
S	5.69390400	3.66796000	2.73425100
S	-5.87158000	0.15955900	2.70456500
S	-1.90733200	0.09622700	2.69184800
S	2.38047800	-0.17441000	2.84900700
S	5.91339600	-0.14210900	2.62582400
H	-5.12077700	-4.72446500	3.20977000
H	-0.91878500	-4.07934700	2.69500900
H	1.97235500	-2.77531300	3.05876300
H	5.25793600	-2.80827000	3.13044700
H	-5.30103500	2.89570300	3.20196200

H	-2.31825600	2.88421200	3.17290400
H	0.78800500	4.17801200	2.69314000
H	5.06694900	4.77414600	3.17673300
H	-5.26504600	-0.94579800	3.17929000
H	-2.26114900	-1.15036600	3.07126700
H	5.15334200	0.82946600	3.16520300
Al	0.71665400	0.11560900	4.37527800
C	-0.00501200	-1.59562000	4.99632300
C	0.00086100	1.87952600	4.80968000
H	-0.87450700	-1.46262900	5.64854700
H	-0.32658400	-2.20664000	4.14922300
H	0.73380300	-2.18439500	5.54875800
H	0.66896400	2.50220400	5.40997800
H	-0.19719600	2.42686400	3.88982700
H	-0.94825100	1.78013200	5.34760300
S	2.82183900	0.26169900	6.02749200
H	3.29740800	1.35842100	5.41101500
H	2.29692000	0.96306900	7.04679900
TS ^{B2-down}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000

Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50200000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000

Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000

H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32268200	7.57590100	-0.14541400
Si	22.32493700	11.42450000	-0.11507300
Si	24.77877400	11.41656200	-0.14440500
Si	22.33350200	3.72940800	-0.13685400
Si	24.77927600	7.57463600	-0.17255700
Si	24.78520900	3.74166200	-0.13728300
Si	30.00717200	7.58089500	-0.09662200

Si	29.98892200	11.42337400	-0.13388200
Si	32.43780500	11.42516700	-0.13278600
Si	29.98140200	3.74765600	-0.14124900
Si	32.48387100	7.58433700	-0.16212700
Si	32.44582300	3.73794800	-0.11067800
S	21.61571100	3.90485200	1.90390100
S	25.20849600	3.70984700	1.98873900
S	29.15465400	3.57961700	1.85362900
S	33.16708800	3.56912500	1.91032900
S	21.58172100	11.61462100	1.89884900
S	25.53502900	11.64712100	1.86987100
S	29.54191000	11.52379800	1.98444100
S	33.14530400	11.24922100	1.91105700
S	21.59558700	7.76198600	1.88217400
S	25.56774200	7.68137000	1.84696500
S	29.92233000	7.50100800	2.04508000
S	33.41303200	7.43963300	1.78494400
H	22.33594200	2.87491600	2.38577000
H	26.54065200	3.52325600	1.87100300
H	29.48916800	4.82648200	2.24765100
H	32.74814600	4.78711600	2.30988700
H	22.16112000	10.49814900	2.37960100
H	25.14901300	10.44132900	2.33150200
H	28.23959800	11.84014900	1.84129600
H	32.51841800	12.35121800	2.36413000
H	22.20442500	6.65720600	2.35535900

H	25.23278500	6.42866200	2.22220800
H	32.65197200	8.38275800	2.37098000
Al	28.35162600	7.63396200	3.63063000
C	27.35907100	6.06245300	4.20535900
C	27.46292800	9.49244500	3.92754200
H	26.43041000	6.31428200	4.72574400
H	27.10149800	5.43019500	3.35288100
H	27.96952300	5.46212100	4.88611100
H	27.79101700	10.43622800	4.37736200
H	27.38470100	9.71734700	2.86034500
H	26.47485600	9.26067400	4.33384000
S	29.86500900	8.24799600	5.42433900
H	30.70976300	8.88573200	4.59435700
H	28.63891000	9.07552300	4.78406400
Im2 ^{B2-down}			
Si	-3.91510000	5.73621200	-1.89120100
Si	-5.83515100	5.73433400	-0.53361500
Si	-3.91131100	1.89612500	-1.89110600
Si	-5.83138100	1.89401000	-0.53348400
Si	-3.91322000	3.81622900	-3.24888800
Si	-0.07520000	5.74020900	-1.89114800
Si	-1.99514200	5.73810200	-0.53357200
Si	-0.07140200	1.90002500	-1.89108200
Si	-1.99125600	1.89817000	-0.53365900
Si	-0.07312000	3.82014100	-3.24887100

Si	-3.90751600	-1.94397300	-1.89108900
Si	-5.82746700	-1.94586400	-0.53370500
Si	-3.90931100	-0.02386300	-3.24900100
Si	-3.90351700	-5.78397200	-1.89118600
Si	-5.82352700	-5.78607800	-0.53359300
Si	-3.90541400	-3.86397300	-3.24888500
Si	-0.06736700	-1.93996500	-1.89103000
Si	-1.98733700	-1.94147600	-0.53348000
Si	-0.06922500	-0.01997700	-3.24885700
Si	-0.06342400	-5.78016600	-1.89107200
Si	-1.98362400	-5.78176300	-0.53368100
Si	-0.06532700	-3.86008900	-3.24886600
Si	3.76498000	5.74402400	-1.89118800
Si	1.84511100	5.74202500	-0.53368900
Si	3.76878400	1.90393300	-1.89110700
Si	1.84914800	1.90157300	-0.53372200
Si	3.76697300	3.82402200	-3.24889300
Si	5.68510800	5.74584000	-0.53360300
Si	5.68902600	1.90583400	-0.53360500
Si	3.77276700	-1.93625000	-1.89110400
Si	1.85291400	-1.93816800	-0.53389100
Si	3.77087700	-0.01607800	-3.24898300
Si	3.77677800	-5.77627000	-1.89119000
Si	1.85670200	-5.77824800	-0.53367400
Si	3.77476500	-3.85615800	-3.24890400
Si	5.69283100	-1.93377700	-0.53330000

Si	5.69649400	-5.77397600	-0.53359700
H	-3.88570600	6.93342300	-2.80249200
H	-1.97786400	6.92573200	0.38751000
H	-7.15270500	1.92873900	-1.22551200
H	-0.07551600	7.00123800	-2.70287100
H	-7.08202200	5.41554700	-1.29198800
H	-5.96443600	6.99132600	0.26111500
H	-3.05051900	3.84392800	-4.45398600
H	-5.32531900	3.82872800	-3.78658600
H	1.09818100	3.77852800	-4.15158600
H	-1.24641900	3.77052800	-4.14818600
H	-3.05821900	-0.01047200	-4.46588600
H	-5.32401900	-0.01397200	-3.78668600
H	1.09588100	-0.00447200	-4.16188600
H	-1.25691900	-0.00617200	-4.13128600
H	1.10158100	-3.80087200	-4.15728600
H	-1.24051900	-3.79637200	-4.14528600
H	3.75487400	6.93992800	-2.80398600
H	5.78408700	6.97872900	0.30641200
H	6.95397800	5.47113800	-1.27049400
H	1.83759000	6.93682500	0.37571900
H	7.01917800	1.94772900	-1.20789100
H	5.18028100	3.83042800	-3.78458600
H	2.90468100	3.85112800	-4.45358600
H	7.01977900	-1.91108100	-1.21569000
H	5.18068100	-0.00227200	-3.79808600

H	2.90478100	0.00012800	-4.45358600
H	1.85119000	-6.97887100	0.36501500
H	3.76947600	-6.96337000	-2.81608900
H	6.95627800	-5.48167900	-1.28099500
H	5.80628300	-7.01607500	0.28651000
H	5.18748100	-3.84597200	-3.78668600
H	2.91188100	-3.86497200	-4.45368600
H	-0.05942100	-7.03057600	-2.71928100
H	-5.93171800	-7.03107200	0.28211400
H	-7.07961700	-5.49727400	-1.28859000
H	-7.14691400	-1.91658100	-1.23059600
H	-3.88501800	-6.96937200	-2.81898600
H	-1.96441700	-6.97917100	0.36961500
H	-3.04321900	-3.87707200	-4.45488600
H	-5.31681900	-3.86687200	-3.79038600
Si	-5.14724200	-0.02351800	0.68443400
Si	-5.12409000	3.82542500	0.71762100
Si	-2.66738700	3.81602100	0.69096200
Si	-5.12933500	-3.87114600	0.68732100
Si	-2.68570500	-0.02609200	0.63024300
Si	-2.67997100	-3.86196700	0.68198700
Si	2.50861500	-0.01660700	0.72505200
Si	2.53418400	3.82752200	0.68722300
Si	4.98259500	3.82626300	0.68841300
Si	2.52513500	-3.85287600	0.68052300
Si	4.98747100	-0.01622400	0.67552700

Si	4.98942900	-3.86362400	0.71084300
S	-5.83781400	-3.68493500	2.72951300
S	-2.25175000	-3.90311100	2.80779800
S	1.70379800	-4.02405600	2.67551600
S	5.71685100	-4.05234800	2.72737700
S	-5.84756400	4.01940700	2.73720400
S	-1.84059600	4.04514600	2.67130200
S	2.10426700	3.99361800	2.79656100
S	5.70117800	3.64546800	2.72395900
S	-5.85872000	0.17228800	2.71240800
S	-1.99420600	-0.04277000	2.73874200
S	2.19569100	-0.07140800	2.84254700
S	5.79258100	-0.17309400	2.67423500
H	-5.12758400	-4.72115600	3.21256100
H	-0.92033300	-4.09491500	2.68468100
H	2.01517200	-2.76921700	3.06500600
H	5.29549500	-2.84266800	3.14839400
H	-5.23979100	2.92179800	3.22843900
H	-2.15542000	2.83990100	3.18009100
H	0.79700400	4.29122500	2.65548200
H	5.07486800	4.74492000	3.18409600
H	-5.25895800	-0.93700600	3.18726900
H	-2.23742700	-1.35590000	2.96923700
H	5.00074000	0.77091000	3.21984200
Al	0.24406400	-0.01040900	3.97236600
C	-0.15485100	-1.65548900	4.93959300

C	-3.79871900	2.16709800	5.49758000
H	-1.09740200	-1.57831400	5.49111400
H	-0.20889800	-2.53941500	4.30291600
H	0.63476500	-1.82815600	5.67819200
H	-4.83743000	2.07232800	5.81569200
H	-3.57484300	3.21210900	5.28062400
H	-3.63860800	1.55832900	4.60576000
S	-0.03038300	1.86818800	5.10261900
H	1.06561400	2.45049400	4.58468300
H	-3.13693900	1.81898300	6.28990400
$P^{B2-down}$			
Si	-3.91510000	5.73620000	-1.89120000
Si	-5.83520000	5.73430000	-0.53360000
Si	-3.91130000	1.89610000	-1.89110000
Si	-5.83140000	1.89400000	-0.53350000
Si	-3.91320000	3.81620000	-3.24890000
Si	-0.07520000	5.74020000	-1.89110000
Si	-1.99510000	5.73810000	-0.53360000
Si	-0.07140000	1.90000000	-1.89110000
Si	-1.99130000	1.89820000	-0.53370000
Si	-0.07310000	3.82010000	-3.24890000
Si	-3.90750000	-1.94400000	-1.89110000
Si	-5.82750000	-1.94590000	-0.53370000
Si	-3.90930000	-0.02390000	-3.24900000
Si	-3.90350000	-5.78400000	-1.89120000

Si	-5.82350000	-5.78610000	-0.53360000
Si	-3.90540000	-3.86400000	-3.24890000
Si	-0.06740000	-1.94000000	-1.89100000
Si	-1.98730000	-1.94150000	-0.53350000
Si	-0.06920000	-0.02000000	-3.24890000
Si	-0.06340000	-5.78020000	-1.89110000
Si	-1.98360000	-5.78180000	-0.53370000
Si	-0.06530000	-3.86010000	-3.24890000
Si	3.76500000	5.74400000	-1.89120000
Si	1.84510000	5.74200000	-0.53370000
Si	3.76880000	1.90390000	-1.89110000
Si	1.84910000	1.90160000	-0.53370000
Si	3.76700000	3.82400000	-3.24890000
Si	5.68510000	5.74580000	-0.53360000
Si	5.68900000	1.90580000	-0.53360000
Si	3.77280000	-1.93630000	-1.89110000
Si	1.85290000	-1.93820000	-0.53390000
Si	3.77090000	-0.01610000	-3.24900000
Si	3.77680000	-5.77630000	-1.89120000
Si	1.85670000	-5.77820000	-0.53370000
Si	3.77480000	-3.85620000	-3.24890000
Si	5.69280000	-1.93380000	-0.53330000
Si	5.69650000	-5.77400000	-0.53360000
H	-3.88570000	6.93340000	-2.80250000
H	-1.97790000	6.92570000	0.38750000
H	-7.15270000	1.92870000	-1.22550000

H	-0.07550000	7.00120000	-2.70290000
H	-7.08200000	5.41550000	-1.29200000
H	-5.96440000	6.99130000	0.26110000
H	-3.05050000	3.84390000	-4.45400000
H	-5.32530000	3.82870000	-3.78660000
H	1.09820000	3.77850000	-4.15160000
H	-1.24640000	3.77050000	-4.14820000
H	-3.05820000	-0.01050000	-4.46590000
H	-5.32400000	-0.01400000	-3.78670000
H	1.09590000	-0.00450000	-4.16190000
H	-1.25690000	-0.00620000	-4.13130000
H	1.10160000	-3.80090000	-4.15730000
H	-1.24050000	-3.79640000	-4.14530000
H	3.75490000	6.93990000	-2.80400000
H	5.78410000	6.97870000	0.30640000
H	6.95400000	5.47110000	-1.27050000
H	1.83760000	6.93680000	0.37570000
H	7.01920000	1.94770000	-1.20790000
H	5.18030000	3.83040000	-3.78460000
H	2.90470000	3.85110000	-4.45360000
H	7.01980000	-1.91110000	-1.21570000
H	5.18070000	-0.00230000	-3.79810000
H	2.90480000	0.00010000	-4.45360000
H	1.85120000	-6.97890000	0.36500000
H	3.76950000	-6.96340000	-2.81610000
H	6.95630000	-5.48170000	-1.28100000

H	5.80630000	-7.01610000	0.28650000
H	5.18750000	-3.84600000	-3.78670000
H	2.91190000	-3.86500000	-4.45370000
H	-0.05940000	-7.03060000	-2.71930000
H	-5.93170000	-7.03110000	0.28210000
H	-7.07960000	-5.49730000	-1.28860000
H	-7.14690000	-1.91660000	-1.23060000
H	-3.88500000	-6.96940000	-2.81900000
H	-1.96440000	-6.97920000	0.36960000
H	-3.04320000	-3.87710000	-4.45490000
H	-5.31680000	-3.86690000	-3.79040000
Si	-5.14679500	-0.02378800	0.68448700
Si	-5.12541800	3.82567400	0.71544200
Si	-2.66845800	3.81588400	0.69275000
Si	-5.12927700	-3.87136700	0.68715500
Si	-2.68389900	-0.02567500	0.63376500
Si	-2.67988500	-3.86192300	0.68184600
Si	2.51012500	-0.01709200	0.72402000
Si	2.53423900	3.82763200	0.68667800
Si	4.98263400	3.82624400	0.68845200
Si	2.52527500	-3.85300600	0.68042300
Si	4.98839300	-0.01623500	0.67502700
Si	4.98949500	-3.86360700	0.71084100
S	-5.83862200	-3.68729800	2.72940800
S	-2.25187500	-3.90025800	2.80735600
S	1.70448600	-4.02687400	2.67520500

S	5.71684500	-4.05189300	2.72741800
S	-5.86199500	4.02038400	2.73026700
S	-1.85319700	4.04628800	2.67845300
S	2.10380300	3.99393000	2.79575000
S	5.70067600	3.64543500	2.72413400
S	-5.87123400	0.16850800	2.70875600
S	-1.99395900	-0.02649500	2.74401500
S	2.20126400	-0.07591400	2.84112800
S	5.79491800	-0.17280600	2.67311500
H	-5.12427800	-4.72051100	3.21287400
H	-0.92073900	-4.09416700	2.68432000
H	2.01762400	-2.77307000	3.06647800
H	5.29607100	-2.84181900	3.14787700
H	-5.26333200	2.91826900	3.22058300
H	-2.17871100	2.84414700	3.18757100
H	0.79639400	4.29087700	2.65588800
H	5.07479300	4.74524000	3.18401600
H	-5.27779000	-0.94359500	3.18413700
H	-2.24191100	-1.33712400	2.98190500
H	5.00284400	0.77040200	3.21968300
Al	0.25324600	-0.01230200	3.97663400
C	-0.14939400	-1.66218000	4.93389100
H	-1.08873200	-1.58762300	5.49066900
H	-0.20761200	-2.54165900	4.29171400
H	0.64360300	-1.84118400	5.66742700
S	0.01141300	1.86108100	5.11845800

H	1.10256000	2.43343500	4.57999800
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P^{B2-up}			
Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600

Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000

H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900

H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31303900	7.57670600	-0.13859500
Si	22.33160800	11.42576800	-0.11137000
Si	24.78600700	11.41817500	-0.13761000
Si	22.33193500	3.72886000	-0.13534600
Si	24.77618800	7.57645300	-0.19004700
Si	24.78281100	3.74082300	-0.13925100
Si	29.97568500	7.58197400	-0.10746400
Si	29.98326500	11.42171700	-0.12544000
Si	32.43677200	11.42750900	-0.13383700
Si	29.98077100	3.74712200	-0.14212700
Si	32.45237600	7.58315800	-0.14862400
Si	32.44562200	3.73727800	-0.11353300
S	21.62319100	3.90942200	1.90799300
S	25.22231900	3.72424900	1.98651400
S	29.15937700	3.56894800	1.85405000
S	33.16144600	3.54867400	1.90745900
S	21.59410000	11.61572700	1.90437200
S	25.59710800	11.65540200	1.84582600
S	29.56250900	11.45279400	1.98860300
S	33.15826200	11.25525200	1.90209300
S	21.59031100	7.76388900	1.88771700
S	25.48523400	7.60277100	1.91542600
S	29.66561500	7.45027600	2.00703500

S	33.24516300	7.41824700	1.85227000
H	22.34710800	2.88250500	2.39089500
H	26.55382900	3.53055100	1.86003200
H	29.44205200	4.83447600	2.23249700
H	32.58016900	4.67223000	2.37171300
H	22.19138900	10.51109600	2.39053000
H	25.26785200	10.45017000	2.34390300
H	28.23794900	11.68336600	1.88706600
H	32.42737200	12.27818700	2.38329600
H	22.18221400	6.64842700	2.35728600
H	25.25949900	6.29294900	2.17650400
H	32.47624000	8.39212500	2.37881200
Al	27.74403100	7.68560600	3.13713300
C	27.30054500	6.09531900	4.17930400
H	26.35535600	6.19670400	4.72155600
H	27.23330400	5.19741300	3.56004700
H	28.08405700	5.92041700	4.92349300
S	27.58615200	9.65070800	4.13920900
H	26.61645500	9.20476400	4.96168800
Im1 ^{B3-up}			
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Si	-5.83782700	5.73159200	-0.58511800
Si	-3.91402700	1.89339200	-1.94251800
Si	-5.83392700	1.89129200	-0.58491800
Si	-3.91592700	3.81349200	-3.30041800

Si	-0.07792700	5.73749200	-1.94271800
Si	-1.99772700	5.73539200	-0.58511800
Si	-0.07402700	1.89739200	-1.94271800
Si	-1.99392700	1.89549200	-0.58511800
Si	-0.07582700	3.81739200	-3.30041800
Si	-3.91022700	-1.94670800	-1.94261800
Si	-5.83012700	-1.94860800	-0.58521800
Si	-3.91202700	-0.02660800	-3.30051800
Si	-3.90622700	-5.78670800	-1.94271800
Si	-5.82622700	-5.78880800	-0.58511800
Si	-3.90812700	-3.86670800	-3.30041800
Si	-0.07002700	-1.94270800	-1.94261800
Si	-1.99002700	-1.94420800	-0.58501800
Si	-0.07192700	-0.02270800	-3.30041800
Si	-0.06612700	-5.78290800	-1.94261800
Si	-1.98632700	-5.78450800	-0.58521800
Si	-0.06802700	-3.86280800	-3.30041800
Si	3.76227300	5.74129200	-1.94271800
Si	1.84237300	5.73939200	-0.58521800
Si	3.76607300	1.90129200	-1.94261800
Si	1.84617300	1.89869200	-0.58521800
Si	3.76427300	3.82129200	-3.30041800
Si	5.68237300	5.74309200	-0.58511800
Si	5.68627300	1.90319200	-0.58501800
Si	3.77007300	-1.93900800	-1.94261800
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Si	3.76817300	-0.01880800	-3.30051800
Si	3.77407300	-5.77900800	-1.94271800
Si	1.85397300	-5.78100800	-0.58521800
Si	3.77207300	-3.85890800	-3.30041800
Si	5.69007300	-1.93640800	-0.58491800
Si	5.69377300	-5.77670800	-0.58511800
H	-3.88842700	6.93069200	-2.85401800
H	-1.98052700	6.92299200	0.33598200
H	-7.15542700	1.92599200	-1.27701800
H	-0.07822700	6.99849200	-2.75441800
H	-7.08472700	5.41279200	-1.34351800
H	-5.96712700	6.98859200	0.20958200
H	-3.05322700	3.84119200	-4.50551800
H	-5.32802700	3.82599200	-3.83811800
H	1.09547300	3.77579200	-4.20311800
H	-1.24912700	3.76779200	-4.19971800
H	-3.06092700	-0.01320800	-4.51741800
H	-5.32672700	-0.01670800	-3.83821800
H	1.09317300	-0.00720800	-4.21341800
H	-1.25962700	-0.00890800	-4.18281800
H	1.09887300	-3.80360800	-4.20881800
H	-1.24322700	-3.79910800	-4.19681800
H	3.75217300	6.93719200	-2.85551800
H	5.78137300	6.97599200	0.25488200
H	6.95127300	5.46839200	-1.32201800
H	1.83487300	6.93409200	0.32418200

H	7.01647300	1.94499200	-1.25941800
H	5.17757300	3.82769200	-3.83611800
H	2.90197300	3.84839200	-4.50511800
H	7.01707300	-1.91380800	-1.26721800
H	5.17797300	-0.00500800	-3.84961800
H	2.90207300	-0.00260800	-4.50511800
H	1.84847300	-6.98160800	0.31348200
H	3.76677300	-6.96610800	-2.86761800
H	6.95357300	-5.48440800	-1.33251800
H	5.80357300	-7.01880800	0.23498200
H	5.18477300	-3.84870800	-3.83821800
H	2.90917300	-3.86770800	-4.50521800
H	-0.06212700	-7.03330800	-2.77081800
H	-5.93442700	-7.03380800	0.23058200
H	-7.08232700	-5.50000800	-1.34011800
H	-7.14962700	-1.91930800	-1.28211800
H	-3.88772700	-6.97210800	-2.87051800
H	-1.96712700	-6.98190800	0.31808200
H	-3.04592700	-3.87980800	-4.50641800
H	-5.31952700	-3.86960800	-3.84191800
Si	-5.13805900	-0.02670800	0.62778900
Si	-5.12609500	3.82200300	0.65958300
Si	-2.66955900	3.81422600	0.63364800
Si	-5.12829400	-3.87373900	0.63532200
Si	-2.67903200	-0.02703700	0.60281500
Si	-2.67652900	-3.86156000	0.63456400

Si	2.53950000	-0.02005800	0.66485400
Si	2.51912400	3.81701600	0.64914500
Si	4.97197000	3.82529300	0.63955500
Si	2.51748500	-3.85591400	0.63027800
Si	5.01435600	-0.01848900	0.61303700
Si	4.98137500	-3.86473800	0.65829900
S	-5.84395600	-3.70308200	2.67767500
S	-2.24891000	-3.90141200	2.76085100
S	1.68794200	-4.02861600	2.62544300
S	5.70135200	-4.01600600	2.68514900
S	-5.86081200	4.01164100	2.67688300
S	-1.85796600	4.03987100	2.61930400
S	2.09154300	3.84602200	2.76466600
S	5.69650700	3.66728200	2.68003400
S	-5.87007100	0.15449400	2.65395700
S	-1.89721100	0.07126100	2.63011300
S	2.38390100	-0.16477300	2.79736300
S	5.91111400	-0.15776700	2.57778100
H	-5.12307200	-4.73421200	3.15602600
H	-0.91795600	-4.09465100	2.63817100
H	1.93489100	-2.75054000	2.98371300
H	5.26770000	-2.79765500	3.06659200
H	-5.26351200	2.90517300	3.15921900
H	-2.13833800	2.80338800	3.07156600
H	0.76320500	4.05727500	2.65846900
H	4.94298800	4.67208500	3.16453400

H	-5.26362300	-0.95254000	3.12477000
H	-2.25650400	-1.17897600	2.99158000
H	5.28026500	0.91844500	3.08690000
S	0.06268100	2.12225100	4.98516400
H	-1.02505800	1.59745400	5.58142600
Al	0.78151900	0.12483500	4.33946100
C	-0.09499300	-1.50782800	4.96579300
H	0.54244100	-2.09264200	5.63575300
H	-0.33902500	-2.15171500	4.11689500
H	-1.02894100	-1.30384800	5.49857200
S	2.85251900	0.20207700	5.95147200
H	2.25953800	-0.10699100	7.11829800
H	3.34164500	-1.03809200	5.76893700
TS ^{B3-up}			
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Si	-5.81950000	5.73790000	-0.53570000
Si	-3.89570000	1.89970000	-1.89310000
Si	-5.81560000	1.89760000	-0.53550000
Si	-3.89760000	3.81980000	-3.25100000
Si	-0.05960000	5.74380000	-1.89330000
Si	-1.97940000	5.74170000	-0.53570000
Si	-0.05570000	1.90370000	-1.89330000
Si	-1.97560000	1.90180000	-0.53570000
Si	-0.05750000	3.82370000	-3.25100000
Si	-3.89190000	-1.94040000	-1.89320000

Si	-5.81180000	-1.94230000	-0.53580000
Si	-3.89370000	-0.02030000	-3.25110000
Si	-3.88790000	-5.78040000	-1.89330000
Si	-5.80790000	-5.78250000	-0.53570000
Si	-3.88980000	-3.86040000	-3.25100000
Si	-0.05170000	-1.93640000	-1.89320000
Si	-1.97170000	-1.93790000	-0.53560000
Si	-0.05360000	-0.01640000	-3.25100000
Si	-0.04780000	-5.77660000	-1.89320000
Si	-1.96800000	-5.77820000	-0.53580000
Si	-0.04970000	-3.85650000	-3.25100000
Si	3.78060000	5.74760000	-1.89330000
Si	1.86070000	5.74570000	-0.53580000
Si	3.78440000	1.90760000	-1.89320000
Si	1.86450000	1.90500000	-0.53580000
Si	3.78260000	3.82760000	-3.25100000
Si	5.70070000	5.74940000	-0.53570000
Si	5.70460000	1.90950000	-0.53560000
Si	3.78840000	-1.93270000	-1.89320000
Si	1.86860000	-1.93460000	-0.53610000
Si	3.78650000	-0.01250000	-3.25110000
Si	3.79240000	-5.77270000	-1.89330000
Si	1.87230000	-5.77470000	-0.53580000
Si	3.79040000	-3.85260000	-3.25100000
Si	5.70840000	-1.93010000	-0.53550000
Si	5.71210000	-5.77040000	-0.53570000

H	-3.87010000	6.93700000	-2.80460000
H	-1.96220000	6.92930000	0.38540000
H	-7.13710000	1.93230000	-1.22760000
H	-0.05990000	7.00480000	-2.70500000
H	-7.06640000	5.41910000	-1.29410000
H	-5.94880000	6.99490000	0.25900000
H	-3.03490000	3.84750000	-4.45610000
H	-5.30970000	3.83230000	-3.78870000
H	1.11380000	3.78210000	-4.15370000
H	-1.23080000	3.77410000	-4.15030000
H	-3.04260000	-0.00690000	-4.46800000
H	-5.30840000	-0.01040000	-3.78880000
H	1.11150000	-0.00090000	-4.16400000
H	-1.24130000	-0.00260000	-4.13340000
H	1.11720000	-3.79730000	-4.15940000
H	-1.22490000	-3.79280000	-4.14740000
H	3.77050000	6.94350000	-2.80610000
H	5.79970000	6.98230000	0.30430000
H	6.96960000	5.47470000	-1.27260000
H	1.85320000	6.94040000	0.37360000
H	7.03480000	1.95130000	-1.21000000
H	5.19590000	3.83400000	-3.78670000
H	2.92030000	3.85470000	-4.45570000
H	7.03540000	-1.90750000	-1.21780000
H	5.19630000	0.00130000	-3.80020000
H	2.92040000	0.00370000	-4.45570000

H	1.86680000	-6.97530000	0.36290000
H	3.78510000	-6.95980000	-2.81820000
H	6.97190000	-5.47810000	-1.28310000
H	5.82190000	-7.01250000	0.28440000
H	5.20310000	-3.84240000	-3.78880000
H	2.92750000	-3.86140000	-4.45580000
H	-0.04380000	-7.02700000	-2.72140000
H	-5.91610000	-7.02750000	0.28000000
H	-7.06400000	-5.49370000	-1.29070000
H	-7.13130000	-1.91300000	-1.23270000
H	-3.86940000	-6.96580000	-2.82110000
H	-1.94880000	-6.97560000	0.36750000
H	-3.02760000	-3.87350000	-4.45700000
H	-5.30120000	-3.86330000	-3.79250000
Si	-5.12222100	-0.02028600	0.67663800
Si	-5.11066500	3.82831000	0.70824400
Si	-2.65558400	3.82061900	0.67874100
Si	-5.10809000	-3.86762300	0.68679300
Si	-2.66523300	-0.02007100	0.64625500
Si	-2.65541700	-3.85362700	0.68573500
Si	2.56136100	-0.01469700	0.71427700
Si	2.53972300	3.82125600	0.69705200
Si	4.99258100	3.83021100	0.69125400
Si	2.54130200	-3.85143400	0.67775500
Si	5.03824300	-0.01096300	0.66553900
Si	5.00534500	-3.85878600	0.71110300

S	-5.81803900	-3.69646400	2.73139800
S	-2.21036800	-3.87700800	2.81262300
S	1.72504800	-4.04185600	2.67696000
S	5.72546200	-4.02913100	2.73246600
S	-5.84615000	4.01704100	2.72528000
S	-1.85235900	4.04253200	2.66862600
S	2.09880800	3.81541900	2.81225400
S	5.70506800	3.65905100	2.73181500
S	-5.84955400	0.16044900	2.70475500
S	-1.87578900	0.06798600	2.67044000
S	2.43072100	-0.22357000	2.85449100
S	5.92916900	-0.15867300	2.62802900
H	-5.09502400	-4.72696400	3.20803800
H	-0.87877100	-4.06085800	2.68112100
H	2.07528900	-2.79812800	3.06837900
H	5.32148900	-2.80511400	3.12936600
H	-5.25253500	2.90820800	3.20653000
H	-2.17257100	2.81447300	3.11617500
H	0.76959800	4.01526600	2.69986500
H	4.97349800	4.68410900	3.20759800
H	-5.24527200	-0.94907300	3.17249500
H	-2.25912300	-1.17726000	3.02571600
H	5.15737900	0.77959200	3.21017500
S	-0.06310200	2.08935200	5.12068300
H	-1.26454100	1.48691200	5.14297100
Al	1.00179400	0.27347300	4.46780800

C	0.00078900	-1.49498900	5.02151000
H	0.29819400	-2.38102400	5.59728900
H	-0.13615400	-1.87237800	4.00275600
H	-0.95857300	-1.17139600	5.43334900
S	2.56485600	-0.21732800	6.20864700
H	1.83208000	0.43535700	7.12810100
H	1.25039400	-1.06237800	5.73250800
Im2 ^{B3-up}			
Si	-3.91780000	5.73350000	-1.94270000
Si	-5.83780000	5.73160000	-0.58510000
Si	-3.91400000	1.89340000	-1.94250000
Si	-5.83390000	1.89130000	-0.58490000
Si	-3.91590000	3.81350000	-3.30040000
Si	-0.07790000	5.73750000	-1.94270000
Si	-1.99770000	5.73540000	-0.58510000
Si	-0.07400000	1.89740000	-1.94270000
Si	-1.99390000	1.89550000	-0.58510000
Si	-0.07580000	3.81740000	-3.30040000
Si	-3.91020000	-1.94670000	-1.94260000
Si	-5.83010000	-1.94860000	-0.58520000
Si	-3.91200000	-0.02660000	-3.30050000
Si	-3.90620000	-5.78670000	-1.94270000
Si	-5.82620000	-5.78880000	-0.58510000
Si	-3.90810000	-3.86670000	-3.30040000
Si	-0.07000000	-1.94270000	-1.94260000

Si	-1.99000000	-1.94420000	-0.58500000
Si	-0.07190000	-0.02270000	-3.30040000
Si	-0.06610000	-5.78290000	-1.94260000
Si	-1.98630000	-5.78450000	-0.58520000
Si	-0.06800000	-3.86280000	-3.30040000
Si	3.76230000	5.74130000	-1.94270000
Si	1.84240000	5.73940000	-0.58520000
Si	3.76610000	1.90130000	-1.94260000
Si	1.84620000	1.89870000	-0.58520000
Si	3.76430000	3.82130000	-3.30040000
Si	5.68240000	5.74310000	-0.58510000
Si	5.68630000	1.90320000	-0.58500000
Si	3.77010000	-1.93900000	-1.94260000
Si	1.85030000	-1.94090000	-0.58550000
Si	3.76820000	-0.01880000	-3.30050000
Si	3.77410000	-5.77900000	-1.94270000
Si	1.85400000	-5.78100000	-0.58520000
Si	3.77210000	-3.85890000	-3.30040000
Si	5.69010000	-1.93640000	-0.58490000
Si	5.69380000	-5.77670000	-0.58510000
H	-3.88840000	6.93070000	-2.85400000
H	-1.98050000	6.92300000	0.33600000
H	-7.15540000	1.92600000	-1.27700000
H	-0.07820000	6.99850000	-2.75440000
H	-7.08470000	5.41280000	-1.34350000
H	-5.96710000	6.98860000	0.20960000

H	-3.05320000	3.84120000	-4.50550000
H	-5.32800000	3.82600000	-3.83810000
H	1.09550000	3.77580000	-4.20310000
H	-1.24910000	3.76780000	-4.19970000
H	-3.06090000	-0.01320000	-4.51740000
H	-5.32670000	-0.01670000	-3.83820000
H	1.09320000	-0.00720000	-4.21340000
H	-1.25960000	-0.00890000	-4.18280000
H	1.09890000	-3.80360000	-4.20880000
H	-1.24320000	-3.79910000	-4.19680000
H	3.75220000	6.93720000	-2.85550000
H	5.78140000	6.97600000	0.25490000
H	6.95130000	5.46840000	-1.32200000
H	1.83490000	6.93410000	0.32420000
H	7.01650000	1.94500000	-1.25940000
H	5.17760000	3.82770000	-3.83610000
H	2.90200000	3.84840000	-4.50510000
H	7.01710000	-1.91380000	-1.26720000
H	5.17800000	-0.00500000	-3.84960000
H	2.90210000	-0.00260000	-4.50510000
H	1.84850000	-6.98160000	0.31350000
H	3.76680000	-6.96610000	-2.86760000
H	6.95360000	-5.48440000	-1.33250000
H	5.80360000	-7.01880000	0.23500000
H	5.18480000	-3.84870000	-3.83820000
H	2.90920000	-3.86770000	-4.50520000

H	-0.06210000	-7.03330000	-2.77080000
H	-5.93440000	-7.03380000	0.23060000
H	-7.08230000	-5.50000000	-1.34010000
H	-7.14960000	-1.91930000	-1.28210000
H	-3.88770000	-6.97210000	-2.87050000
H	-1.96710000	-6.98190000	0.31810000
H	-3.04590000	-3.87980000	-4.50640000
H	-5.31950000	-3.86960000	-3.84190000
Si	-5.14527100	-0.02662700	0.63529700
Si	-5.13206100	3.82234500	0.66111800
Si	-2.67811500	3.81418000	0.63487600
Si	-5.12862500	-3.87428300	0.63891600
Si	-2.68233200	-0.02608200	0.57360300
Si	-2.67579700	-3.86207400	0.63988800
Si	2.51356900	-0.02212200	0.65327000
Si	2.51879800	3.81673800	0.64819900
Si	4.97303200	3.82432300	0.64065300
Si	2.51703900	-3.85625700	0.63700600
Si	4.99015700	-0.01867400	0.62234000
Si	4.98357600	-3.86623500	0.66145600
S	-5.84289700	-3.68381800	2.68001100
S	-2.26838600	-3.83531500	2.76800500
S	1.68941000	-4.06401400	2.62469300
S	5.71273600	-4.05399800	2.67748000
S	-5.86880300	4.01020100	2.67723100
S	-1.87492500	4.04002400	2.62426700

S	2.07622600	3.83484800	2.76126100
S	5.68609400	3.65178400	2.67960300
S	-5.83553400	0.16262800	2.67174400
S	-1.97235600	-0.01142900	2.68421300
S	2.19732800	-0.17186400	2.77051800
S	5.78383800	-0.17593400	2.62442900
H	-5.12449800	-4.71120300	3.16991400
H	-0.92218100	-3.92586800	2.69624800
H	2.07175100	-2.85165100	3.07683700
H	5.28419700	-2.84785700	3.10154100
H	-5.27281800	2.90360300	3.16081400
H	-2.21335000	2.83298300	3.11240700
H	0.75948300	4.09879500	2.64220800
H	4.94907100	4.67148700	3.15861800
H	-5.23084300	-0.94915300	3.13615900
H	-2.21931000	-1.32043800	2.94120000
H	5.00702400	0.78704700	3.15860600
S	0.04556900	1.95426400	4.95114200
H	-0.97535700	1.48460200	5.69347200
Al	0.27346000	0.05423500	3.85451700
C	-3.94592200	-1.35150500	5.57900700
H	-5.02993400	-1.42492800	5.67274300
H	-3.58733000	-2.08812700	4.85792500
H	-3.67751800	-0.34759600	5.24626300
S	-0.06964700	-1.81824900	5.00021700
H	-0.58819700	-1.21237700	6.08238400

H	-3.48776700	-1.55192700	6.54708300
p ^{B3-up}			
Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900

Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000

H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600

H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31425700	7.57626800	-0.13653400
Si	22.33000100	11.42571700	-0.11153800
Si	24.78427300	11.41750700	-0.13784900
Si	22.33227100	3.72833600	-0.13551400
Si	24.77967900	7.57639900	-0.19359200
Si	24.78564400	3.74157900	-0.13113900
Si	29.97705300	7.58164600	-0.12197400
Si	29.98167600	11.41995100	-0.12450900
Si	32.43560300	11.42744100	-0.13262300
Si	29.97746000	3.74689500	-0.13578900
Si	32.45327800	7.58314200	-0.14911000
Si	32.44349200	3.73715800	-0.11187400
S	21.60383900	3.91099900	1.90041000
S	25.19085800	3.77390900	1.99782300
S	29.15014900	3.54336600	1.85256800
S	33.16291600	3.54906400	1.90779200
S	21.59217600	11.61621400	1.90394300
S	25.58944400	11.64509100	1.85074000
S	29.54252900	11.43928000	1.98902800
S	33.15053500	11.25549000	1.90573700
S	21.59936300	7.76436700	1.89210500
S	25.48878400	7.59186400	1.92097600
S	29.65740500	7.42981300	1.99355400
S	33.23702700	7.41795000	1.85481100

H	22.32838200	2.88946900	2.39335100
H	26.53328000	3.64222200	1.92186000
H	29.51028500	4.76579600	2.29571500
H	32.57736300	4.66847800	2.37663600
H	22.18743100	10.51054200	2.39016800
H	25.25159000	10.43855100	2.34021100
H	28.22525600	11.70147900	1.87246000
H	32.41347600	12.27468700	2.38566500
H	22.18634800	6.64453000	2.35803400
H	25.23812200	6.28477100	2.18402600
H	32.47787300	8.40245300	2.37544100
Al	27.73778900	7.66222000	3.08320900
S	27.52576200	9.56371800	4.17980500
H	26.49959500	9.10102100	4.91895300
S	27.39142400	5.79435900	4.23756300
H	27.06886200	6.40827700	5.38853600
Im1 ^{B3-down}			
Si	-3.91780000	5.73350000	-1.94270000
Si	-5.83780000	5.73160000	-0.58510000
Si	-3.91400000	1.89340000	-1.94250000
Si	-5.83390000	1.89130000	-0.58490000
Si	-3.91590000	3.81350000	-3.30040000
Si	-0.07790000	5.73750000	-1.94270000
Si	-1.99770000	5.73540000	-0.58510000
Si	-0.07400000	1.89740000	-1.94270000

Si	-1.99390000	1.89550000	-0.58510000
Si	-0.07580000	3.81740000	-3.30040000
Si	-3.91020000	-1.94670000	-1.94260000
Si	-5.83010000	-1.94860000	-0.58520000
Si	-3.91200000	-0.02660000	-3.30050000
Si	-3.90620000	-5.78670000	-1.94270000
Si	-5.82620000	-5.78880000	-0.58510000
Si	-3.90810000	-3.86670000	-3.30040000
Si	-0.07000000	-1.94270000	-1.94260000
Si	-1.99000000	-1.94420000	-0.58500000
Si	-0.07190000	-0.02270000	-3.30040000
Si	-0.06610000	-5.78290000	-1.94260000
Si	-1.98630000	-5.78450000	-0.58520000
Si	-0.06800000	-3.86280000	-3.30040000
Si	3.76230000	5.74130000	-1.94270000
Si	1.84240000	5.73940000	-0.58520000
Si	3.76610000	1.90130000	-1.94260000
Si	1.84620000	1.89870000	-0.58520000
Si	3.76430000	3.82130000	-3.30040000
Si	5.68240000	5.74310000	-0.58510000
Si	5.68630000	1.90320000	-0.58500000
Si	3.77010000	-1.93900000	-1.94260000
Si	1.85030000	-1.94090000	-0.58550000
Si	3.76820000	-0.01880000	-3.30050000
Si	3.77410000	-5.77900000	-1.94270000
Si	1.85400000	-5.78100000	-0.58520000

Si	3.77210000	-3.85890000	-3.30040000
Si	5.69010000	-1.93640000	-0.58490000
Si	5.69380000	-5.77670000	-0.58510000
H	-3.88840000	6.93070000	-2.85400000
H	-1.98050000	6.92300000	0.33600000
H	-7.15540000	1.92600000	-1.27700000
H	-0.07820000	6.99850000	-2.75440000
H	-7.08470000	5.41280000	-1.34350000
H	-5.96710000	6.98860000	0.20960000
H	-3.05320000	3.84120000	-4.50550000
H	-5.32800000	3.82600000	-3.83810000
H	1.09550000	3.77580000	-4.20310000
H	-1.24910000	3.76780000	-4.19970000
H	-3.06090000	-0.01320000	-4.51740000
H	-5.32670000	-0.01670000	-3.83820000
H	1.09320000	-0.00720000	-4.21340000
H	-1.25960000	-0.00890000	-4.18280000
H	1.09890000	-3.80360000	-4.20880000
H	-1.24320000	-3.79910000	-4.19680000
H	3.75220000	6.93720000	-2.85550000
H	5.78140000	6.97600000	0.25490000
H	6.95130000	5.46840000	-1.32200000
H	1.83490000	6.93410000	0.32420000
H	7.01650000	1.94500000	-1.25940000
H	5.17760000	3.82770000	-3.83610000
H	2.90200000	3.84840000	-4.50510000

H	7.01710000	-1.91380000	-1.26720000
H	5.17800000	-0.00500000	-3.84960000
H	2.90210000	-0.00260000	-4.50510000
H	1.84850000	-6.98160000	0.31350000
H	3.76680000	-6.96610000	-2.86760000
H	6.95360000	-5.48440000	-1.33250000
H	5.80360000	-7.01880000	0.23500000
H	5.18480000	-3.84870000	-3.83820000
H	2.90920000	-3.86770000	-4.50520000
H	-0.06210000	-7.03330000	-2.77080000
H	-5.93440000	-7.03380000	0.23060000
H	-7.08230000	-5.50000000	-1.34010000
H	-7.14960000	-1.91930000	-1.28210000
H	-3.88770000	-6.97210000	-2.87050000
H	-1.96710000	-6.98190000	0.31810000
H	-3.04590000	-3.87980000	-4.50640000
H	-5.31950000	-3.86960000	-3.84190000
Si	-5.13690300	-0.02797100	0.62628500
Si	-5.12725100	3.82224700	0.66049400
Si	-2.67020100	3.81437800	0.63354100
Si	-5.12807800	-3.87381100	0.63546600
Si	-2.67738200	-0.02727100	0.60419900
Si	-2.67617900	-3.86158300	0.63484200
Si	2.53723700	-0.01978600	0.66692300
Si	2.51945800	3.81718500	0.64877400
Si	4.97134100	3.82529000	0.63855200

Si	2.51722900	-3.85543600	0.63039400
Si	5.01291000	-0.01927700	0.60938400
Si	4.98069800	-3.86449500	0.65817000
S	-5.84422100	-3.70354500	2.67752200
S	-2.25026000	-3.90058200	2.76109500
S	1.69040500	-4.02445000	2.62584100
S	5.69889500	-4.01062400	2.68598400
S	-5.87075800	4.01449400	2.67404700
S	-1.85280300	4.05460000	2.61350200
S	2.10082200	3.85836800	2.76794600
S	5.69630200	3.67973500	2.68347900
S	-5.87977800	0.14591300	2.64990900
S	-1.89561000	0.07195900	2.62948700
S	2.39978800	-0.13375400	2.80242600
S	5.92517800	-0.14948200	2.57059100
H	-5.12376800	-4.73494000	3.15595800
H	-0.91894300	-4.09064100	2.64004700
H	1.96589900	-2.75566700	2.99595800
H	5.24742100	-2.79933300	3.06858700
H	-5.41777300	2.82538800	3.11777000
H	-2.16284100	2.83697200	3.09581100
H	0.77216800	4.07176200	2.66986700
H	4.95636800	4.69989300	3.15646900
H	-5.26545300	-0.95342100	3.12799300
H	-2.25273500	-1.17956200	2.98899100
H	5.31419200	0.94572600	3.06250100

S	0.08064600	2.13803900	4.93552000
H	-0.89478300	1.63530000	5.71631500
Al	0.78644100	0.11494900	4.34670100
C	-0.08379500	-1.51692200	4.96976800
H	0.56219500	-2.09417200	5.63797100
H	-0.33255300	-2.16206300	4.12357000
H	-1.01321500	-1.31278300	5.51005700
S	2.77149000	0.23026400	6.07720200
H	3.24849600	1.35308100	5.51113100
H	3.67333600	-0.55297100	5.45525600
TS ^{B2-down}			
Si	-3.89950000	5.73980000	-1.89330000
Si	-5.81950000	5.73790000	-0.53570000
Si	-3.89570000	1.89970000	-1.89310000
Si	-5.81560000	1.89760000	-0.53550000
Si	-3.89760000	3.81980000	-3.25100000
Si	-0.05960000	5.74380000	-1.89330000
Si	-1.97940000	5.74170000	-0.53570000
Si	-0.05570000	1.90370000	-1.89330000
Si	-1.97560000	1.90180000	-0.53570000
Si	-0.05750000	3.82370000	-3.25100000
Si	-3.89190000	-1.94040000	-1.89320000
Si	-5.81180000	-1.94230000	-0.53580000
Si	-3.89370000	-0.02030000	-3.25110000
Si	-3.88790000	-5.78040000	-1.89330000

Si	-5.80790000	-5.78250000	-0.53570000
Si	-3.88980000	-3.86040000	-3.25100000
Si	-0.05170000	-1.93640000	-1.89320000
Si	-1.97170000	-1.93790000	-0.53560000
Si	-0.05360000	-0.01640000	-3.25100000
Si	-0.04780000	-5.77660000	-1.89320000
Si	-1.96800000	-5.77820000	-0.53580000
Si	-0.04970000	-3.85650000	-3.25100000
Si	3.78060000	5.74760000	-1.89330000
Si	1.86070000	5.74570000	-0.53580000
Si	3.78440000	1.90760000	-1.89320000
Si	1.86450000	1.90500000	-0.53580000
Si	3.78260000	3.82760000	-3.25100000
Si	5.70070000	5.74940000	-0.53570000
Si	5.70460000	1.90950000	-0.53560000
Si	3.78840000	-1.93270000	-1.89320000
Si	1.86860000	-1.93460000	-0.53610000
Si	3.78650000	-0.01250000	-3.25110000
Si	3.79240000	-5.77270000	-1.89330000
Si	1.87230000	-5.77470000	-0.53580000
Si	3.79040000	-3.85260000	-3.25100000
Si	5.70840000	-1.93010000	-0.53550000
Si	5.71210000	-5.77040000	-0.53570000
H	-3.87010000	6.93700000	-2.80460000
H	-1.96220000	6.92930000	0.38540000
H	-7.13710000	1.93230000	-1.22760000

H	-0.05990000	7.00480000	-2.70500000
H	-7.06640000	5.41910000	-1.29410000
H	-5.94880000	6.99490000	0.25900000
H	-3.03490000	3.84750000	-4.45610000
H	-5.30970000	3.83230000	-3.78870000
H	1.11380000	3.78210000	-4.15370000
H	-1.23080000	3.77410000	-4.15030000
H	-3.04260000	-0.00690000	-4.46800000
H	-5.30840000	-0.01040000	-3.78880000
H	1.11150000	-0.00090000	-4.16400000
H	-1.24130000	-0.00260000	-4.13340000
H	1.11720000	-3.79730000	-4.15940000
H	-1.22490000	-3.79280000	-4.14740000
H	3.77050000	6.94350000	-2.80610000
H	5.79970000	6.98230000	0.30430000
H	6.96960000	5.47470000	-1.27260000
H	1.85320000	6.94040000	0.37360000
H	7.03480000	1.95130000	-1.21000000
H	5.19590000	3.83400000	-3.78670000
H	2.92030000	3.85470000	-4.45570000
H	7.03540000	-1.90750000	-1.21780000
H	5.19630000	0.00130000	-3.80020000
H	2.92040000	0.00370000	-4.45570000
H	1.86680000	-6.97530000	0.36290000
H	3.78510000	-6.95980000	-2.81820000
H	6.97190000	-5.47810000	-1.28310000

H	5.82190000	-7.01250000	0.28440000
H	5.20310000	-3.84240000	-3.78880000
H	2.92750000	-3.86140000	-4.45580000
H	-0.04380000	-7.02700000	-2.72140000
H	-5.91610000	-7.02750000	0.28000000
H	-7.06400000	-5.49370000	-1.29070000
H	-7.13130000	-1.91300000	-1.23270000
H	-3.86940000	-6.96580000	-2.82110000
H	-1.94880000	-6.97560000	0.36750000
H	-3.02760000	-3.87350000	-4.45700000
H	-5.30120000	-3.86330000	-3.79250000
Si	-5.12118200	-0.02028000	0.67706900
Si	-5.11039200	3.82836400	0.70847300
Si	-2.65501000	3.82060500	0.67900500
Si	-5.10801100	-3.86758300	0.68685000
Si	-2.66336800	-0.02017000	0.64861800
Si	-2.65515800	-3.85339100	0.68600400
Si	2.55934100	-0.01451300	0.71182100
Si	2.53983100	3.82078600	0.69700900
Si	4.99249500	3.83116200	0.69079700
Si	2.53952200	-3.85205300	0.67823400
Si	5.03580400	-0.01065000	0.66482200
Si	5.00362000	-3.85849400	0.70960900
S	-5.81765600	-3.69588500	2.73126000
S	-2.20938800	-3.87466000	2.81260800
S	1.71924000	-4.05273600	2.67509500

S	5.72564200	-4.01266900	2.73347900
S	-5.84545800	4.01786300	2.72533500
S	-1.84993900	4.04292800	2.66794700
S	2.10385400	3.80460800	2.81215200
S	5.70810000	3.66742500	2.73145700
S	-5.84887900	0.16129200	2.70475600
S	-1.87176100	0.06955600	2.67187800
S	2.40496900	-0.25694800	2.84679700
S	5.91625400	-0.13927900	2.63634400
H	-5.09403800	-4.72577700	3.20830800
H	-0.87829700	-4.06093300	2.67959800
H	2.03620300	-2.79872500	3.06209700
H	5.31953500	-2.78390200	3.11240500
H	-5.25198000	2.90919500	3.20713500
H	-2.17343700	2.81644700	3.11755300
H	0.77320200	3.99799100	2.70523900
H	4.97266800	4.68968300	3.20723500
H	-5.24389400	-0.94739100	3.17357200
H	-2.25387400	-1.17532900	3.02961700
H	5.16060800	0.83461300	3.18080600
S	-0.04822500	2.10417800	5.12759500
H	-1.25165400	1.50584000	5.13835200
Al	1.01128600	0.28910100	4.48091600
C	0.00198900	-1.46603100	5.06426400
H	0.29877300	-2.34355700	5.65272500
H	-0.12679600	-1.85535500	4.04840600

H	-0.96193000	-1.14165000	5.46395300
S	2.52112300	-0.12235600	6.28015200
H	3.33491400	-0.93673700	5.58275400
H	1.21726400	-0.98627600	5.81109900
Im2 ^{B3-down}			
Si	-3.91780000	5.73350000	-1.94270000
Si	-5.83780000	5.73160000	-0.58510000
Si	-3.91400000	1.89340000	-1.94250000
Si	-5.83390000	1.89130000	-0.58490000
Si	-3.91590000	3.81350000	-3.30040000
Si	-0.07790000	5.73750000	-1.94270000
Si	-1.99770000	5.73540000	-0.58510000
Si	-0.07400000	1.89740000	-1.94270000
Si	-1.99390000	1.89550000	-0.58510000
Si	-0.07580000	3.81740000	-3.30040000
Si	-3.91020000	-1.94670000	-1.94260000
Si	-5.83010000	-1.94860000	-0.58520000
Si	-3.91200000	-0.02660000	-3.30050000
Si	-3.90620000	-5.78670000	-1.94270000
Si	-5.82620000	-5.78880000	-0.58510000
Si	-3.90810000	-3.86670000	-3.30040000
Si	-0.07000000	-1.94270000	-1.94260000
Si	-1.99000000	-1.94420000	-0.58500000
Si	-0.07190000	-0.02270000	-3.30040000
Si	-0.06610000	-5.78290000	-1.94260000

Si	-1.98630000	-5.78450000	-0.58520000
Si	-0.06800000	-3.86280000	-3.30040000
Si	3.76230000	5.74130000	-1.94270000
Si	1.84240000	5.73940000	-0.58520000
Si	3.76610000	1.90130000	-1.94260000
Si	1.84620000	1.89870000	-0.58520000
Si	3.76430000	3.82130000	-3.30040000
Si	5.68240000	5.74310000	-0.58510000
Si	5.68630000	1.90320000	-0.58500000
Si	3.77010000	-1.93900000	-1.94260000
Si	1.85030000	-1.94090000	-0.58550000
Si	3.76820000	-0.01880000	-3.30050000
Si	3.77410000	-5.77900000	-1.94270000
Si	1.85400000	-5.78100000	-0.58520000
Si	3.77210000	-3.85890000	-3.30040000
Si	5.69010000	-1.93640000	-0.58490000
Si	5.69380000	-5.77670000	-0.58510000
H	-3.88840000	6.93070000	-2.85400000
H	-1.98050000	6.92300000	0.33600000
H	-7.15540000	1.92600000	-1.27700000
H	-0.07820000	6.99850000	-2.75440000
H	-7.08470000	5.41280000	-1.34350000
H	-5.96710000	6.98860000	0.20960000
H	-3.05320000	3.84120000	-4.50550000
H	-5.32800000	3.82600000	-3.83810000
H	1.09550000	3.77580000	-4.20310000

H	-1.24910000	3.76780000	-4.19970000
H	-3.06090000	-0.01320000	-4.51740000
H	-5.32670000	-0.01670000	-3.83820000
H	1.09320000	-0.00720000	-4.21340000
H	-1.25960000	-0.00890000	-4.18280000
H	1.09890000	-3.80360000	-4.20880000
H	-1.24320000	-3.79910000	-4.19680000
H	3.75220000	6.93720000	-2.85550000
H	5.78140000	6.97600000	0.25490000
H	6.95130000	5.46840000	-1.32200000
H	1.83490000	6.93410000	0.32420000
H	7.01650000	1.94500000	-1.25940000
H	5.17760000	3.82770000	-3.83610000
H	2.90200000	3.84840000	-4.50510000
H	7.01710000	-1.91380000	-1.26720000
H	5.17800000	-0.00500000	-3.84960000
H	2.90210000	-0.00260000	-4.50510000
H	1.84850000	-6.98160000	0.31350000
H	3.76680000	-6.96610000	-2.86760000
H	6.95360000	-5.48440000	-1.33250000
H	5.80360000	-7.01880000	0.23500000
H	5.18480000	-3.84870000	-3.83820000
H	2.90920000	-3.86770000	-4.50520000
H	-0.06210000	-7.03330000	-2.77080000
H	-5.93440000	-7.03380000	0.23060000
H	-7.08230000	-5.50000000	-1.34010000

H	-7.14960000	-1.91930000	-1.28210000
H	-3.88770000	-6.97210000	-2.87050000
H	-1.96710000	-6.98190000	0.31810000
H	-3.04590000	-3.87980000	-4.50640000
H	-5.31950000	-3.86960000	-3.84190000
Si	-5.14693200	-0.02637000	0.63748300
Si	-5.13201300	3.82243200	0.66146100
Si	-2.67840500	3.81574600	0.63485900
Si	-5.12989100	-3.87372200	0.63862600
Si	-2.68147700	-0.02647000	0.57789900
Si	-2.67925800	-3.86166600	0.63233400
Si	2.51028100	-0.02225300	0.65941700
Si	2.52082100	3.81716100	0.64597100
Si	4.97444100	3.82430800	0.63989600
Si	2.52315500	-3.85733100	0.63232400
Si	4.98793200	-0.01863200	0.62451600
Si	4.98829800	-3.86615800	0.66016300
S	-5.82799200	-3.68245200	2.68377200
S	-2.23978200	-3.87438000	2.75727000
S	1.72558800	-4.07299200	2.63440800
S	5.71843900	-4.05606400	2.67511000
S	-5.86749200	4.01123500	2.67750600
S	-1.87370000	4.06290100	2.61917400
S	2.08705500	3.82760500	2.75919700
S	5.68920700	3.64881500	2.67758400
S	-5.85266900	0.16791100	2.66757900

S	-1.96139800	0.04239500	2.68209900
S	2.18074700	-0.20999500	2.77487600
S	5.77955100	-0.17911000	2.62702400
H	-5.10435400	-4.70850500	3.16938500
H	-0.91269700	-4.09549700	2.63213300
H	2.10378900	-2.85171300	3.06853700
H	5.30122400	-2.84593400	3.09897100
H	-5.27130000	2.90495100	3.16167900
H	-2.21581400	2.86455600	3.12506800
H	0.76876900	4.08995100	2.65126900
H	4.95550500	4.67002100	3.15836300
H	-5.25465000	-0.94219100	3.14354100
H	-2.27245200	-1.22809700	3.02651400
H	4.99822300	0.77809400	3.16494500
S	0.09310200	2.07200600	4.92082800
H	-0.89321400	1.60099700	5.70938800
Al	0.28763800	0.13805800	3.88781400
C	-3.96795700	-1.34827600	5.54590900
H	-5.03231500	-1.36333200	5.78301000
H	-3.75882800	-2.07200200	4.75532600
H	-3.67921400	-0.34896100	5.21742500
S	-0.17572000	-1.55278200	5.23869300
H	-0.08143200	-2.49080400	4.27913100
H	-3.38653000	-1.61829500	6.42583600
p ^{B3-down}			

Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50200000	-1.35790000

Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000

H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31362100	7.57653500	-0.13580900

Si	22.32990900	11.42573900	-0.11134000
Si	24.78356100	11.41928300	-0.13825800
Si	22.33256400	3.72885000	-0.13460300
Si	24.78000000	7.57640000	-0.19099000
Si	24.78375600	3.74137000	-0.13914700
Si	29.97251100	7.58134100	-0.11463600
Si	29.98367500	11.42055500	-0.12691500
Si	32.43702400	11.42739800	-0.13336400
Si	29.98386000	3.74591500	-0.14066400
Si	32.45040300	7.58310100	-0.14634800
Si	32.44845800	3.73713500	-0.11328300
S	21.62675900	3.91451500	1.90840900
S	25.22669700	3.73017900	1.98504300
S	29.18857800	3.54542600	1.86428600
S	33.16858800	3.54729700	1.90540200
S	21.59297200	11.61578100	1.90410400
S	25.58963900	11.67056600	1.84467500
S	29.55266000	11.43337300	1.98655100
S	33.15305800	11.25176700	1.90382900
S	21.59267300	7.76604000	1.89021200
S	25.49333300	7.64184000	1.91815200
S	29.63772800	7.39433200	2.00010500
S	33.23047300	7.41425400	1.85853400
H	22.35605500	2.89323600	2.39533500
H	26.55303400	3.50785100	1.85362200
H	29.54328100	4.78239000	2.27452300

H	32.58874900	4.66974200	2.37403700
H	22.18927500	10.51070700	2.39051300
H	25.24979900	10.47285500	2.35313500
H	28.23458000	11.69696500	1.88012600
H	32.41968200	12.27273900	2.38556000
H	22.17906200	6.64809600	2.36100600
H	25.18811300	6.36806200	2.25553100
H	32.46548400	8.39260500	2.38231100
Al	27.74710200	7.74778300	3.11580600
S	27.56287100	9.68720000	4.13981100
H	26.57828200	9.22475500	4.93533600
S	27.29916300	6.06187700	4.47711600
H	27.37872600	5.12161200	3.51882700

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Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500

Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600

Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
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H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000

H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31425700	7.57626800	-0.13653400
Si	22.33000100	11.42571700	-0.11153800
Si	24.78427300	11.41750700	-0.13784900
Si	22.33227100	3.72833600	-0.13551400
Si	24.77967900	7.57639900	-0.19359200
Si	24.78564400	3.74157900	-0.13113900
Si	29.97705300	7.58164600	-0.12197400
Si	29.98167600	11.41995100	-0.12450900
Si	32.43560300	11.42744100	-0.13262300
Si	29.97746000	3.74689500	-0.13578900
Si	32.45327800	7.58314200	-0.14911000

Si	32.44349200	3.73715800	-0.11187400
S	21.60383900	3.91099900	1.90041000
S	25.19085800	3.77390900	1.99782300
S	29.15014900	3.54336600	1.85256800
S	33.16291600	3.54906400	1.90779200
S	21.59217600	11.61621400	1.90394300
S	25.58944400	11.64509100	1.85074000
S	29.54252900	11.43928000	1.98902800
S	33.15053500	11.25549000	1.90573700
S	21.59936300	7.76436700	1.89210500
S	25.48878400	7.59186400	1.92097600
S	29.65740500	7.42981300	1.99355400
S	33.23702700	7.41795000	1.85481100
H	22.32838200	2.88946900	2.39335100
H	26.53328000	3.64222200	1.92186000
H	29.51028500	4.76579600	2.29571500
H	32.57736300	4.66847800	2.37663600
H	22.18743100	10.51054200	2.39016800
H	25.25159000	10.43855100	2.34021100
H	28.22525600	11.70147900	1.87246000
H	32.41347600	12.27468700	2.38566500
H	22.18634800	6.64453000	2.35803400
H	25.23812200	6.28477100	2.18402600
H	32.47787300	8.40245300	2.37544100
Al	27.73778900	7.66222000	3.08320900
S	27.52576200	9.56371800	4.17980500

H	26.49959500	9.10102100	4.91895300
S	27.39142400	5.79435900	4.23756300
H	27.06886200	6.40827700	5.38853600
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Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000

Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
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Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
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H	24.40860000	11.44430000	-5.27810000
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H	26.21860000	3.80400000	-4.96940000
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H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
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H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000

H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32466800	7.57536300	-0.13448900
Si	22.33443600	11.42512000	-0.11203700
Si	24.79096400	11.41988700	-0.13775800
Si	22.32975700	3.72850500	-0.13894600
Si	24.79366500	7.57585900	-0.16443900
Si	24.78050200	3.73735100	-0.13926800
Si	29.97741500	7.58409000	-0.12970700
Si	29.98498400	11.42196500	-0.12757200
Si	32.43733900	11.42761200	-0.13363000
Si	29.97880300	3.74716400	-0.13669200
Si	32.45086500	7.58247200	-0.14659300
Si	32.44452300	3.73648700	-0.11237200
S	21.59665400	3.89968900	1.89582700
S	25.17797500	3.70197800	1.97915000
S	29.15414100	3.56536200	1.85765100
S	33.16842400	3.54448700	1.90630700
S	21.60175800	11.60716900	1.90660500
S	25.59893400	11.69119800	1.84494100
S	29.54700700	11.45855400	1.98594400
S	33.15282400	11.25404000	1.90503300
S	21.60342000	7.75258500	1.89334400
S	25.43612700	7.78471800	1.93753800

S	29.59124000	7.45413700	1.98819600
S	33.21001500	7.41095700	1.86678600
H	22.31725600	2.87147500	2.38063200
H	26.51032000	3.50672900	1.88823600
H	29.47129600	4.81408800	2.25885300
H	32.58136200	4.66048600	2.38063000
H	22.19854200	10.49766500	2.38285700
H	25.26556400	10.48637800	2.34054900
H	28.23471800	11.74490200	1.87097900
H	32.41476500	12.27161400	2.38682500
H	22.21594600	6.64479000	2.35629900
H	25.77830300	6.51075100	2.83355100
H	32.48182400	8.42713700	2.36955300
Al	27.62352500	7.92554000	2.87759900
S	27.61128600	9.65061700	4.24916800
H	26.42265600	9.32187800	4.78887400
S	26.98624100	5.95968900	3.97262500
H	26.44507600	6.56266400	5.04659200
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Si	-5.76610600	5.73913500	-0.50875300
Si	-3.84230600	1.90093500	-1.86625300
Si	-5.76230600	1.89883500	-0.50865300
Si	-3.84420600	3.82103500	-3.22405300
Si	-0.00620600	5.74503500	-1.86635300

Si	-1.92610600	5.74293500	-0.50875300
Si	-0.00240600	1.90483500	-1.86625300
Si	-1.92220600	1.90293500	-0.50885300
Si	-0.00410600	3.82493500	-3.22405300
Si	-3.83850600	-1.93916500	-1.86625300
Si	-5.75840600	-1.94106500	-0.50885300
Si	-3.84030600	-0.01906500	-3.22415300
Si	-3.83450600	-5.77916500	-1.86635300
Si	-5.75450600	-5.78126500	-0.50875300
Si	-3.83640600	-3.85916500	-3.22405300
Si	0.00169400	-1.93516500	-1.86625300
Si	-1.91830600	-1.93666500	-0.50865300
Si	-0.00020600	-0.01516500	-3.22405300
Si	0.00559400	-5.77536500	-1.86625300
Si	-1.91460600	-5.77696500	-0.50885300
Si	0.00369400	-3.85526500	-3.22405300
Si	3.83399400	5.74883500	-1.86635300
Si	1.91409400	5.74683500	-0.50885300
Si	3.83779400	1.90873500	-1.86625300
Si	1.91809400	1.90643500	-0.50895300
Si	3.83599400	3.82883500	-3.22405300
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Si	3.84179400	-1.93146500	-1.86625300
Si	1.92189400	-1.93336500	-0.50905300
Si	3.83989400	-0.01126500	-3.22415300

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Si	5.76549400	-5.76916500	-0.50875300
H	-3.81670600	6.93823500	-2.77765300
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H	-7.08370600	1.93353500	-1.20065300
H	-0.00650600	7.00603500	-2.67805300
H	-7.01300600	5.42033500	-1.26715300
H	-5.89540600	6.99613500	0.28594700
H	-2.98150600	3.84873500	-4.42915300
H	-5.25630600	3.83353500	-3.76175300
H	1.16719400	3.78333500	-4.12675300
H	-1.17740600	3.77533500	-4.12335300
H	-2.98920600	-0.00566500	-4.44105300
H	-5.25500600	-0.00916500	-3.76185300
H	1.16489400	0.00033500	-4.13705300
H	-1.18790600	-0.00136500	-4.10645300
H	1.17059400	-3.79606500	-4.13245300
H	-1.17150600	-3.79156500	-4.12045300
H	3.82389400	6.94473500	-2.77915300
H	5.85309400	6.98353500	0.33124700
H	7.02299400	5.47593500	-1.24565300
H	1.90659400	6.94163500	0.40054700
H	7.08819400	1.95253500	-1.18305300

H	5.24929400	3.83523500	-3.75975300
H	2.97369400	3.85593500	-4.42875300
H	7.08879400	-1.90626500	-1.19085300
H	5.24969400	0.00253500	-3.77325300
H	2.97379400	0.00493500	-4.42875300
H	1.92019400	-6.97406500	0.38984700
H	3.83849400	-6.95856500	-2.79125300
H	7.02529400	-5.47686500	-1.25615300
H	5.87529400	-7.01126500	0.31134700
H	5.25649400	-3.84116500	-3.76185300
H	2.98089400	-3.86016500	-4.42885300
H	0.00959400	-7.02576500	-2.69445300
H	-5.86270600	-7.02626500	0.30694700
H	-7.01060600	-5.49246500	-1.26375300
H	-7.07790600	-1.91176500	-1.20575300
H	-3.81600600	-6.96456500	-2.79415300
H	-1.89540600	-6.97436500	0.39444700
H	-2.97420600	-3.87226500	-4.43005300
H	-5.24780600	-3.86206500	-3.76555300
Si	-5.04664800	-0.01782700	0.70715700
Si	-5.05372000	3.82947100	0.73492700
Si	-2.59678200	3.82134000	0.70679300
Si	-5.05546200	-3.86374600	0.71657800
Si	-2.57082800	-0.01310400	0.71415000
Si	-2.60464200	-3.85870200	0.70460900
Si	2.57143400	-0.01369800	0.71409100

Si	2.59160600	3.82512800	0.72645400
Si	5.04530600	3.83267000	0.71605200
Si	2.60253300	-3.84840900	0.70805900
Si	5.04675800	-0.01280900	0.70760700
Si	5.06498000	-3.85895200	0.73270600
S	-5.74643200	-3.68657200	2.76401800
S	-2.10558800	-4.07499700	2.81769000
S	1.84356400	-4.03038200	2.73327200
S	5.80103900	-4.05047000	2.74746900
S	-5.78458000	4.01164900	2.75373700
S	-1.79502000	4.02344200	2.70140700
S	2.15836100	3.83919200	2.84047100
S	5.76702700	3.65815900	2.75309300
S	-5.77832500	0.14343300	2.73552100
S	-2.07468500	0.02244200	2.81384700
S	2.09102300	-0.15383800	2.81365800
S	5.76639300	-0.18537600	2.73702000
H	-5.12036500	-4.79268600	3.20810600
H	-0.86613200	-4.55836600	2.60543000
H	2.22847500	-2.79439900	3.11545700
H	5.22587900	-2.92849400	3.22180300
H	-5.19083500	2.89823400	3.22506200
H	-2.10074500	2.77549800	3.10615000
H	0.83316400	4.06585900	2.73174900
H	5.03078100	4.67632400	3.23632300
H	-5.02352100	-0.86006200	3.22383800

H	-0.87921300	-2.51201800	4.20046000
H	5.01783700	0.82249100	3.22778400
Al	0.03407700	0.24688900	3.54907200
S	0.10598600	1.82446800	5.09508600
H	-1.20011800	1.71105600	5.40205300
S	-0.05289600	-1.79193700	5.00255200
H	-1.05732500	-1.35568600	5.78405200
P ^{B4}			
Si	23.54399900	13.33659800	-2.71529800
Si	21.62400400	13.33468300	-1.35769300
Si	23.54778300	9.49647800	-2.71517600
Si	21.62785200	9.49433900	-1.35763900
Si	23.54590100	11.41659800	-4.07300500
Si	27.38389900	13.34059700	-2.71530200
Si	25.46399800	13.33847600	-1.35769700
Si	27.38770500	9.50035700	-2.71526200
Si	25.46777000	9.49839000	-1.35775900
Si	27.38599900	11.42049700	-4.07300600
Si	23.55157900	5.65640200	-2.71516200
Si	21.63176900	5.65452600	-1.35781200
Si	23.54980000	7.57649900	-4.07309300
Si	23.55559900	1.81640500	-2.71530000
Si	21.63561000	1.81431800	-1.35770000
Si	23.55370100	3.73640100	-4.07300400
Si	27.39179200	5.66044900	-2.71525600

Si	25.47165600	5.65902100	-1.35759400
Si	27.38989800	7.58039700	-4.07299900
Si	27.39569800	1.82020300	-2.71520200
Si	25.47549900	1.81864600	-1.35779400
Si	27.39380400	3.74029800	-4.07299900
Si	31.22410100	13.34440000	-2.71529800
Si	29.30419400	13.34238200	-1.35779900
Si	31.22791600	9.50431000	-2.71517400
Si	29.30829600	9.50196900	-1.35789200
Si	31.22610100	11.42440000	-4.07300200
Si	33.14420000	13.34619400	-1.35769700
Si	33.14807400	9.50619500	-1.35769800
Si	31.23190700	5.66409900	-2.71518900
Si	29.31206600	5.66228300	-1.35804300
Si	31.22999700	7.58430000	-4.07310000
Si	31.23589900	1.82410200	-2.71530000
Si	29.31579700	1.82211400	-1.35779300
Si	31.23390100	3.74420100	-4.07300200
Si	33.15187100	5.66661900	-1.35742000
Si	33.15560100	1.82640500	-1.35769700
H	23.57339900	14.53380200	-3.62659800
H	25.48130500	14.52609700	-0.43659700
H	20.30640600	9.52908900	-2.04961100
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01589800	-2.11609900
H	21.49469800	14.59169800	-0.56299700

H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030100	-3.62809900
H	33.24320100	14.57909900	-0.51769900
H	34.41310000	13.07150000	-2.09460000
H	29.29669700	14.53719800	-0.44839800
H	34.47829600	9.54809400	-2.03200800
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889800	5.68930400	-2.03980300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31029800	0.62150200	-0.45909800
H	31.22860000	0.63699900	-3.64019900
H	34.41540000	2.11870000	-2.10510000
H	33.26540100	0.58430100	-0.53759900
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000

H	27.39970000	0.56979900	-3.54339900
H	21.52740000	0.56930100	-0.54199800
H	20.37949900	2.10310200	-2.11269800
H	20.31220200	5.68380900	-2.05470300
H	23.57409900	0.63099800	-3.64309800
H	25.49470800	0.62120400	-0.45449500
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.34588000	7.57579800	-0.13848600
Si	22.32887200	11.42471300	-0.11369200
Si	24.78585400	11.41551500	-0.14036100
Si	22.33996000	3.72925600	-0.13400300
Si	24.82363700	7.58267900	-0.14498300
Si	24.79620500	3.74012500	-0.12424200
Si	29.97037900	7.58168100	-0.14667700
Si	29.97897400	11.42072800	-0.12941800
Si	32.43255100	11.42737800	-0.13086700
Si	29.98596800	3.74599800	-0.13787600
Si	32.44250700	7.58104900	-0.14181800
Si	32.44830300	3.73540600	-0.11440600
S	21.61371600	3.90371900	1.90214300
S	25.23662600	3.68596100	1.98940600
S	29.18836300	3.55954600	1.86608900
S	33.17813900	3.53479400	1.90158600
S	21.59363900	11.61211700	1.90287800
S	25.56140600	11.63823500	1.87045700

S	29.47421300	11.45605800	1.97951600
S	33.12614800	11.24776600	1.91547100
S	21.62115300	7.76206900	1.88789100
S	25.37133800	7.68420100	1.95530900
S	29.45457200	7.49731900	1.96392000
S	33.16130700	7.39005500	1.88390600
H	22.35691800	2.89227000	2.38901600
H	26.55848900	3.45080500	1.85474600
H	29.37752400	4.84656300	2.21903700
H	32.58201100	4.63956300	2.38969700
H	22.17446400	10.49319200	2.37701800
H	25.13519800	10.44551300	2.33049600
H	28.21477700	11.90702200	1.82052400
H	32.36491100	12.24776400	2.39873900
H	22.25917300	6.67552000	2.36634200
H	32.51339400	8.46818500	2.36747000
Al	27.44188400	8.16858700	2.51135300
S	27.48101600	9.13448900	4.46127800
H	26.15040000	9.04223400	4.63763900

P^{B2-up}			
Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100

Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400
Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200

Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200
H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900

H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31303900	7.57670600	-0.13859500
Si	22.33160800	11.42576800	-0.11137000
Si	24.78600700	11.41817500	-0.13761000
Si	22.33193500	3.72886000	-0.13534600
Si	24.77618800	7.57645300	-0.19004700

Si	24.78281100	3.74082300	-0.13925100
Si	29.97568500	7.58197400	-0.10746400
Si	29.98326500	11.42171700	-0.12544000
Si	32.43677200	11.42750900	-0.13383700
Si	29.98077100	3.74712200	-0.14212700
Si	32.45237600	7.58315800	-0.14862400
Si	32.44562200	3.73727800	-0.11353300
S	21.62319100	3.90942200	1.90799300
S	25.22231900	3.72424900	1.98651400
S	29.15937700	3.56894800	1.85405000
S	33.16144600	3.54867400	1.90745900
S	21.59410000	11.61572700	1.90437200
S	25.59710800	11.65540200	1.84582600
S	29.56250900	11.45279400	1.98860300
S	33.15826200	11.25525200	1.90209300
S	21.59031100	7.76388900	1.88771700
S	25.48523400	7.60277100	1.91542600
S	29.66561500	7.45027600	2.00703500
S	33.24516300	7.41824700	1.85227000
H	22.34710800	2.88250500	2.39089500
H	26.55382900	3.53055100	1.86003200
H	29.44205200	4.83447600	2.23249700
H	32.58016900	4.67223000	2.37171300
H	22.19138900	10.51109600	2.39053000
H	25.26785200	10.45017000	2.34390300
H	28.23794900	11.68336600	1.88706600

H	32.42737200	12.27818700	2.38329600
H	22.18221400	6.64842700	2.35728600
H	25.25949900	6.29294900	2.17650400
H	32.47624000	8.39212500	2.37881200
Al	27.74403100	7.68560600	3.13713300
C	27.30054500	6.09531900	4.17930400
H	26.35535600	6.19670400	4.72155600
H	27.23330400	5.19741300	3.56004700
H	28.08405700	5.92041700	4.92349300
S	27.58615200	9.65070800	4.13920900
H	26.61645500	9.20476400	4.96168800
TS ^{B5}			
Si	23.54400000	13.33660000	-2.71530000
Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000

Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50200000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000
Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000

H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
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H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000

H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.33725500	7.57513200	-0.14159000
Si	22.31679500	11.42472200	-0.11663800
Si	24.76903100	11.42584100	-0.14790800
Si	22.34008200	3.73003700	-0.13096000
Si	24.80402100	7.58072700	-0.16120100
Si	24.79475000	3.74009900	-0.12813000
Si	29.96615300	7.57376100	-0.11757900
Si	29.97430200	11.41858300	-0.12436300
Si	32.43005500	11.42789800	-0.13084700
Si	29.99352000	3.74429700	-0.14568200
Si	32.44385700	7.58335600	-0.14524900
Si	32.45336900	3.73772600	-0.11691300
S	21.63425100	3.90896100	1.91142100
S	25.25589800	3.69840400	1.98391600

S	29.21459500	3.51626300	1.85914200
S	33.17914000	3.55827900	1.90231200
S	21.55650400	11.59959100	1.89457500
S	25.49534200	11.76500500	1.85414400
S	29.49898400	11.43693700	1.98712300
S	33.13463900	11.26058000	1.91305400
S	21.63910900	7.73081100	1.90023700
S	25.40069300	7.47179600	1.94730200
S	29.58212700	7.44261600	1.98953500
S	33.21675700	7.42209900	1.86540200
H	22.37161800	2.88818200	2.38786000
H	26.56700800	3.41506300	1.83787000
H	29.58330600	4.73724600	2.29774100
H	32.60102800	4.68446200	2.36386900
H	21.86822100	10.34977400	2.28929200
H	24.74864000	10.83484200	2.47585400
H	28.19154200	11.73106800	1.84837800
H	32.38757400	12.27502300	2.38799900
H	22.40494600	6.73157800	2.38190200
H	25.92095500	8.77548500	2.70008000
H	32.47720700	8.42854000	2.37122100
Al	27.56852600	7.19308200	2.92388400
C	27.43291400	5.76908000	4.24236600
H	26.47380000	5.82482000	4.76573100
H	27.50779700	4.76835200	3.81388200
H	28.23048200	5.87272100	4.98483100

S	27.09385800	9.28092800	3.89157600
H	26.34377500	8.75344500	4.87801100
Im1 ^{B5}			
Si	-3.84340000	5.74880000	-1.81770000
Si	-5.76340000	5.74690000	-0.46010000
Si	-3.83960000	1.90870000	-1.81760000
Si	-5.75960000	1.90660000	-0.46000000
Si	-3.84150000	3.82880000	-3.17540000
Si	-0.00350000	5.75280000	-1.81770000
Si	-1.92340000	5.75070000	-0.46010000
Si	0.00030000	1.91260000	-1.81760000
Si	-1.91950000	1.91070000	-0.46020000
Si	-0.00140000	3.83270000	-3.17540000
Si	-3.83580000	-1.93140000	-1.81760000
Si	-5.75570000	-1.93330000	-0.46020000
Si	-3.83760000	-0.01130000	-3.17550000
Si	-3.83180000	-5.77140000	-1.81770000
Si	-5.75180000	-5.77350000	-0.46010000
Si	-3.83370000	-3.85140000	-3.17540000
Si	0.00440000	-1.92740000	-1.81760000
Si	-1.91560000	-1.92890000	-0.46000000
Si	0.00250000	-0.00740000	-3.17540000
Si	0.00830000	-5.76760000	-1.81760000
Si	-1.91190000	-5.76920000	-0.46020000
Si	0.00640000	-3.84750000	-3.17540000

Si	3.83670000	5.75660000	-1.81770000
Si	1.91680000	5.75460000	-0.46020000
Si	3.84050000	1.91650000	-1.81760000
Si	1.92080000	1.91420000	-0.46030000
Si	3.83870000	3.83660000	-3.17540000
Si	5.75680000	5.75840000	-0.46010000
Si	5.76070000	1.91840000	-0.46010000
Si	3.84450000	-1.92370000	-1.81760000
Si	1.92460000	-1.92560000	-0.46040000
Si	3.84260000	-0.00350000	-3.17550000
Si	3.84850000	-5.76370000	-1.81770000
Si	1.92840000	-5.76570000	-0.46020000
Si	3.84650000	-3.84360000	-3.17540000
Si	5.76450000	-1.92120000	-0.45980000
Si	5.76820000	-5.76140000	-0.46010000
H	-3.81400000	6.94600000	-2.72900000
H	-1.90610000	6.93830000	0.46100000
H	-7.08100000	1.94130000	-1.15200000
H	-0.00380000	7.01380000	-2.62940000
H	-7.01030000	5.42810000	-1.21850000
H	-5.89270000	7.00390000	0.33460000
H	-2.97880000	3.85650000	-4.38050000
H	-5.25360000	3.84130000	-3.71310000
H	1.16990000	3.79110000	-4.07810000
H	-1.17470000	3.78310000	-4.07470000
H	-2.98650000	0.00210000	-4.39240000

H	-5.25230000	-0.00140000	-3.71320000
H	1.16760000	0.00810000	-4.08840000
H	-1.18520000	0.00640000	-4.05780000
H	1.17330000	-3.78830000	-4.08380000
H	-1.16880000	-3.78380000	-4.07180000
H	3.82660000	6.95250000	-2.73050000
H	5.85580000	6.99130000	0.37990000
H	7.02570000	5.48370000	-1.19700000
H	1.90930000	6.94940000	0.44920000
H	7.09090000	1.96030000	-1.13440000
H	5.25200000	3.84300000	-3.71110000
H	2.97640000	3.86370000	-4.38010000
H	7.09150000	-1.89850000	-1.14220000
H	5.25240000	0.01030000	-3.72460000
H	2.97650000	0.01270000	-4.38010000
H	1.92290000	-6.96630000	0.43850000
H	3.84120000	-6.95080000	-2.74260000
H	7.02800000	-5.46910000	-1.20750000
H	5.87800000	-7.00350000	0.36000000
H	5.25920000	-3.83340000	-3.71320000
H	2.98360000	-3.85240000	-4.38020000
H	0.01230000	-7.01800000	-2.64580000
H	-5.86000000	-7.01850000	0.35560000
H	-7.00790000	-5.48470000	-1.21510000
H	-7.07520000	-1.90400000	-1.15710000
H	-3.81330000	-6.95680000	-2.74550000

H	-1.89270000	-6.96660000	0.44310000
H	-2.97150000	-3.86450000	-4.38140000
H	-5.24510000	-3.85430000	-3.71690000
Si	-5.03570800	-0.01466200	0.75280100
Si	-5.05752300	3.83662900	0.78235700
Si	-2.58769000	3.83318200	0.77212700
Si	-5.04733100	-3.85587800	0.76709200
Si	-2.55620700	-0.00966000	0.77573100
Si	-2.59282600	-3.84909400	0.76716900
Si	2.57076900	-0.00451500	0.77338100
Si	2.57758100	3.82875900	0.74486400
Si	5.04018900	3.84104700	0.78096000
Si	2.60912100	-3.83912600	0.75506900
Si	5.05069200	-0.00543700	0.75595000
Si	5.06754500	-3.85123800	0.77950700
S	-5.75835100	-3.67360700	2.80472400
S	-2.12998900	-3.92733200	2.87776200
S	1.83901400	-3.99424500	2.77137200
S	5.79879600	-4.04276000	2.79661900
S	-5.79676400	3.98863900	2.81028600
S	-1.91316900	4.04592100	2.83336600
S	1.75654800	3.83700000	2.76822500
S	5.64287900	3.75134300	2.86786700
S	-5.78057100	0.10572200	2.78444900
S	-2.09008000	0.04706000	2.86111100
S	2.04968800	0.02295500	2.85596000

S	5.81827900	-0.19357600	2.76528000
H	-5.13255100	-4.77749100	3.25509700
H	-0.83137500	-4.25121000	2.71847000
H	2.19782400	-2.75258100	3.16033700
H	5.21028800	-2.92955500	3.27504200
H	-5.62731100	2.68966600	3.13230900
H	-3.15294900	4.00111500	3.36457000
H	1.54266100	5.16418800	2.83592100
H	4.43465300	4.10460600	3.34914700
H	-4.81869500	-0.67362300	3.31745300
H	1.18136500	2.01486700	4.96828500
H	5.21260800	0.90950500	3.24595700
Al	-0.03546000	-0.40830600	3.64659100
C	0.02060000	-1.77085900	5.03516500
H	-0.85067000	-1.66229200	5.68825700
H	0.00398900	-2.79004100	4.64708700
H	0.92134500	-1.66310900	5.64846400
S	-0.09716700	1.62840300	5.13600800
H	-0.56977000	2.45654200	4.17221000
p^{B5}			
Si	-3.84640000	5.74340000	-1.76960000
Si	-5.76640000	5.74150000	-0.41200000
Si	-3.84260000	1.90330000	-1.76950000
Si	-5.76260000	1.90120000	-0.41190000
Si	-3.84450000	3.82340000	-3.12730000

Si	-0.00650000	5.74740000	-1.76960000
Si	-1.92640000	5.74530000	-0.41200000
Si	-0.00270000	1.90720000	-1.76950000
Si	-1.92250000	1.90530000	-0.41210000
Si	-0.00440000	3.82730000	-3.12730000
Si	-3.83880000	-1.93680000	-1.76950000
Si	-5.75870000	-1.93870000	-0.41210000
Si	-3.84060000	-0.01670000	-3.12740000
Si	-3.83480000	-5.77680000	-1.76960000
Si	-5.75480000	-5.77890000	-0.41200000
Si	-3.83670000	-3.85680000	-3.12730000
Si	0.00140000	-1.93280000	-1.76950000
Si	-1.91860000	-1.93430000	-0.41190000
Si	-0.00050000	-0.01280000	-3.12730000
Si	0.00530000	-5.77300000	-1.76950000
Si	-1.91490000	-5.77460000	-0.41210000
Si	0.00340000	-3.85290000	-3.12730000
Si	3.83370000	5.75120000	-1.76960000
Si	1.91380000	5.74920000	-0.41210000
Si	3.83750000	1.91110000	-1.76950000
Si	1.91780000	1.90880000	-0.41220000
Si	3.83570000	3.83120000	-3.12730000
Si	5.75380000	5.75300000	-0.41200000
Si	5.75770000	1.91300000	-0.41200000
Si	3.84150000	-1.92910000	-1.76950000
Si	1.92160000	-1.93100000	-0.41230000

Si	3.83960000	-0.00890000	-3.12740000
Si	3.84550000	-5.76910000	-1.76960000
Si	1.92540000	-5.77110000	-0.41210000
Si	3.84350000	-3.84900000	-3.12730000
Si	5.76150000	-1.92660000	-0.41170000
Si	5.76520000	-5.76680000	-0.41200000
H	-3.81700000	6.94060000	-2.68090000
H	-1.90910000	6.93290000	0.50910000
H	-7.08400000	1.93590000	-1.10390000
H	-0.00680000	7.00840000	-2.58130000
H	-7.01330000	5.42270000	-1.17040000
H	-5.89570000	6.99850000	0.38270000
H	-2.98180000	3.85110000	-4.33240000
H	-5.25660000	3.83590000	-3.66500000
H	1.16690000	3.78570000	-4.03000000
H	-1.17770000	3.77770000	-4.02660000
H	-2.98950000	-0.00330000	-4.34430000
H	-5.25530000	-0.00680000	-3.66510000
H	1.16460000	0.00270000	-4.04030000
H	-1.18820000	0.00100000	-4.00970000
H	1.17030000	-3.79370000	-4.03570000
H	-1.17180000	-3.78920000	-4.02370000
H	3.82360000	6.94710000	-2.68240000
H	5.85280000	6.98590000	0.42800000
H	7.02270000	5.47830000	-1.14890000
H	1.90630000	6.94400000	0.49730000

H	7.08790000	1.95490000	-1.08630000
H	5.24900000	3.83760000	-3.66300000
H	2.97340000	3.85830000	-4.33200000
H	7.08850000	-1.90390000	-1.09410000
H	5.24940000	0.00490000	-3.67650000
H	2.97350000	0.00730000	-4.33200000
H	1.91990000	-6.97170000	0.48660000
H	3.83820000	-6.95620000	-2.69450000
H	7.02500000	-5.47450000	-1.15940000
H	5.87500000	-7.00890000	0.40810000
H	5.25620000	-3.83880000	-3.66510000
H	2.98060000	-3.85780000	-4.33210000
H	0.00930000	-7.02340000	-2.59770000
H	-5.86300000	-7.02390000	0.40370000
H	-7.01090000	-5.49010000	-1.16700000
H	-7.07820000	-1.90940000	-1.10900000
H	-3.81630000	-6.96220000	-2.69740000
H	-1.89570000	-6.97200000	0.49120000
H	-2.97450000	-3.86990000	-4.33330000
H	-5.24810000	-3.85970000	-3.66880000
Si	-5.02723800	-0.01933900	0.80834600
Si	-5.06977700	3.83104900	0.82960200
Si	-2.61127600	3.81947400	0.80862200
Si	-5.05130300	-3.86364200	0.81162700
Si	-2.54159300	-0.00475900	0.81737900
Si	-2.59523300	-3.85159000	0.82068300

Si	2.57589500	-0.00560800	0.80605300
Si	2.57845200	3.81670000	0.80388400
Si	5.03714500	3.83212000	0.82314800
Si	2.59440200	-3.84377100	0.80847900
Si	5.04773100	-0.01343300	0.80175700
Si	5.05710200	-3.85809100	0.83121900
S	-5.77761200	-3.69062800	2.84718700
S	-2.16605100	-3.88758600	2.93587200
S	1.79044700	-3.97332800	2.81502700
S	5.78898500	-4.06172000	2.84617900
S	-5.83122800	4.01332500	2.83781600
S	-1.89667700	4.00734700	2.84580700
S	1.84445800	3.75081800	2.86530300
S	5.68789600	3.64998500	2.88156700
S	-5.75590200	0.13833500	2.84025200
S	-1.94211100	0.14340900	2.88609600
S	2.05247100	0.01749300	2.90276600
S	5.75438800	-0.19502600	2.83426200
H	-5.05348900	-4.71976700	3.32536400
H	-0.83580600	-4.07021800	2.80802800
H	1.95137500	-2.66863000	3.11781200
H	5.19546000	-2.95544200	3.33382300
H	-5.49148700	2.77458500	3.24549800
H	-2.62589900	2.98919800	3.34258900
H	1.02468000	4.80922600	2.75345600
H	4.87527700	4.61494300	3.35301100

H	-4.98328700	-0.84650600	3.33973100
H	4.99711100	0.80630300	3.32422300
Al	0.07716800	0.87581200	3.46260800
C	0.05908900	1.69671100	5.21789300
H	1.07588800	1.83928600	5.58953800
H	-0.43254700	2.67210300	5.19004400
H	-0.48909500	1.07027300	5.92718000

P^{B3-up}			
Si	23.54399800	13.33660400	-2.71530000
Si	21.62398800	13.33470900	-1.35771600
Si	23.54779800	9.49651100	-2.71521100
Si	21.62776700	9.49441200	-1.35764100
Si	23.54590000	11.41659700	-4.07300600
Si	27.38390600	13.34059800	-2.71529700
Si	25.46398600	13.33849100	-1.35771100
Si	27.38774300	9.50038600	-2.71515400
Si	25.46793200	9.49846800	-1.35784400
Si	27.38599700	11.42050800	-4.07299500
Si	23.55160000	5.65640500	-2.71518900
Si	21.63171400	5.65451600	-1.35777200
Si	23.54980000	7.57649300	-4.07310100
Si	23.55559800	1.81640400	-2.71529900
Si	21.63561100	1.81431100	-1.35769500
Si	23.55370000	3.73639500	-4.07299400

Si	27.39181000	5.66041800	-2.71521400
Si	25.47180000	5.65887800	-1.35762200
Si	27.38988800	7.58040100	-4.07299400
Si	27.39569400	1.82020400	-2.71519900
Si	25.47550500	1.81862600	-1.35778800
Si	27.39381300	3.74030100	-4.07300600
Si	31.22410200	13.34439600	-2.71529900
Si	29.30421500	13.34236300	-1.35779300
Si	31.22786800	9.50425800	-2.71521000
Si	29.30816300	9.50202700	-1.35786400
Si	31.22609300	11.42439600	-4.07300900
Si	33.14419500	13.34619500	-1.35769900
Si	33.14811100	9.50619200	-1.35766600
Si	31.23189500	5.66411900	-2.71520200
Si	29.31203100	5.66220000	-1.35797300
Si	31.23000600	7.58430600	-4.07308300
Si	31.23590100	1.82409700	-2.71530000
Si	29.31583000	1.82211700	-1.35780700
Si	31.23389400	3.74421100	-4.07301500
Si	33.15193800	5.66659700	-1.35741600
Si	33.15561400	1.82638800	-1.35771600
H	23.57340100	14.53380200	-3.62659800
H	25.48130200	14.52609900	-0.43659900
H	20.30640500	9.52909800	-2.04960900
H	27.38360300	14.60160300	-3.52699500
H	20.37710000	13.01590300	-2.11610200

H	21.49469900	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400100	14.54030200	-3.62809800
H	33.24319500	14.57910100	-0.51770000
H	34.41310100	13.07150100	-2.09459900
H	29.29670000	14.53719700	-0.44839600
H	34.47829700	9.54809500	-2.03200700
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889300	5.68930900	-2.03981300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030200	0.62150000	-0.45910000
H	31.22859800	0.63700000	-3.64020000
H	34.41539900	2.11869700	-2.10510300
H	33.26540100	0.58429900	-0.53760100
H	32.64660000	3.75440000	-4.61080000

H	30.37100000	3.73540000	-5.27780000
H	27.39969600	0.56979800	-3.54339700
H	21.52740400	0.56930000	-0.54200000
H	20.37949900	2.10310100	-2.11269800
H	20.31219600	5.68379800	-2.05469200
H	23.57409900	0.63100000	-3.64309900
H	25.49470600	0.62120300	-0.45449600
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.31425700	7.57626800	-0.13653400
Si	22.33000100	11.42571700	-0.11153800
Si	24.78427300	11.41750700	-0.13784900
Si	22.33227100	3.72833600	-0.13551400
Si	24.77967900	7.57639900	-0.19359200
Si	24.78564400	3.74157900	-0.13113900
Si	29.97705300	7.58164600	-0.12197400
Si	29.98167600	11.41995100	-0.12450900
Si	32.43560300	11.42744100	-0.13262300
Si	29.97746000	3.74689500	-0.13578900
Si	32.45327800	7.58314200	-0.14911000
Si	32.44349200	3.73715800	-0.11187400
S	21.60383900	3.91099900	1.90041000
S	25.19085800	3.77390900	1.99782300
S	29.15014900	3.54336600	1.85256800
S	33.16291600	3.54906400	1.90779200
S	21.59217600	11.61621400	1.90394300

S	25.58944400	11.64509100	1.85074000
S	29.54252900	11.43928000	1.98902800
S	33.15053500	11.25549000	1.90573700
S	21.59936300	7.76436700	1.89210500
S	25.48878400	7.59186400	1.92097600
S	29.65740500	7.42981300	1.99355400
S	33.23702700	7.41795000	1.85481100
H	22.32838200	2.88946900	2.39335100
H	26.53328000	3.64222200	1.92186000
H	29.51028500	4.76579600	2.29571500
H	32.57736300	4.66847800	2.37663600
H	22.18743100	10.51054200	2.39016800
H	25.25159000	10.43855100	2.34021100
H	28.22525600	11.70147900	1.87246000
H	32.41347600	12.27468700	2.38566500
H	22.18634800	6.64453000	2.35803400
H	25.23812200	6.28477100	2.18402600
H	32.47787300	8.40245300	2.37544100
Al	27.73778900	7.66222000	3.08320900
S	27.52576200	9.56371800	4.17980500
H	26.49959500	9.10102100	4.91895300
S	27.39142400	5.79435900	4.23756300
H	27.06886200	6.40827700	5.38853600
TS ^{B6}			
Si	23.54400000	13.33660000	-2.71530000

Si	21.62400000	13.33470000	-1.35770000
Si	23.54780000	9.49650000	-2.71520000
Si	21.62780000	9.49440000	-1.35760000
Si	23.54590000	11.41660000	-4.07300000
Si	27.38390000	13.34060000	-2.71530000
Si	25.46400000	13.33850000	-1.35770000
Si	27.38770000	9.50040000	-2.71520000
Si	25.46790000	9.49850000	-1.35780000
Si	27.38600000	11.42050000	-4.07300000
Si	23.55160000	5.65640000	-2.71520000
Si	21.63170000	5.65450000	-1.35780000
Si	23.54980000	7.57650000	-4.07310000
Si	23.55560000	1.81640000	-2.71530000
Si	21.63560000	1.81430000	-1.35770000
Si	23.55370000	3.73640000	-4.07300000
Si	27.39180000	5.66040000	-2.71520000
Si	25.47180000	5.65890000	-1.35760000
Si	27.38990000	7.58040000	-4.07300000
Si	27.39570000	1.82020000	-2.71520000
Si	25.47550000	1.81860000	-1.35780000
Si	27.39380000	3.74030000	-4.07300000
Si	31.22410000	13.34440000	-2.71530000
Si	29.30420000	13.34240000	-1.35780000
Si	31.22790000	9.50430000	-2.71520000
Si	29.30820000	9.50200000	-1.35790000
Si	31.22610000	11.42440000	-4.07300000

Si	33.14420000	13.34620000	-1.35770000
Si	33.14810000	9.50620000	-1.35770000
Si	31.23190000	5.66410000	-2.71520000
Si	29.31200000	5.66220000	-1.35800000
Si	31.23000000	7.58430000	-4.07310000
Si	31.23590000	1.82410000	-2.71530000
Si	29.31580000	1.82210000	-1.35780000
Si	31.23390000	3.74420000	-4.07300000
Si	33.15190000	5.66660000	-1.35740000
Si	33.15560000	1.82640000	-1.35770000
H	23.57340000	14.53380000	-3.62660000
H	25.48130000	14.52610000	-0.43660000
H	20.30640000	9.52910000	-2.04960000
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01590000	-2.11610000
H	21.49470000	14.59170000	-0.56300000
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000
H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000

H	31.21400000	14.54030000	-3.62810000
H	33.24320000	14.57910000	-0.51770000
H	34.41310000	13.07150000	-2.09460000
H	29.29670000	14.53720000	-0.44840000
H	34.47830000	9.54810000	-2.03200000
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47890000	5.68930000	-2.03980000
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31030000	0.62150000	-0.45910000
H	31.22860000	0.63700000	-3.64020000
H	34.41540000	2.11870000	-2.10510000
H	33.26540000	0.58430000	-0.53760000
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56980000	-3.54340000
H	21.52740000	0.56930000	-0.54200000
H	20.37950000	2.10310000	-2.11270000
H	20.31220000	5.68380000	-2.05470000
H	23.57410000	0.63100000	-3.64310000
H	25.49470000	0.62120000	-0.45450000
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.32290800	7.57542700	-0.13977100
Si	22.33621300	11.42489500	-0.11027500

Si	24.79427200	11.42179100	-0.13256800
Si	22.33186100	3.72929500	-0.13620100
Si	24.78852000	7.57829200	-0.17016900
Si	24.78268700	3.74092900	-0.13930500
Si	29.97140700	7.58201800	-0.12308800
Si	29.98053500	11.42061200	-0.12407700
Si	32.43449300	11.42757900	-0.13219400
Si	29.98975600	3.74513900	-0.14390600
Si	32.44647500	7.58252700	-0.14503200
Si	32.45167600	3.73699600	-0.11608900
S	21.61714300	3.89904300	1.90501700
S	25.22426600	3.70948400	1.97776500
S	29.20646600	3.53936800	1.86448800
S	33.17945700	3.54792300	1.90142900
S	21.60098100	11.60569700	1.90750400
S	25.60166000	11.74111300	1.84316800
S	29.53106700	11.44451400	1.98848000
S	33.14859200	11.25321800	1.90699900
S	21.60210100	7.75240100	1.88763100
S	25.38827000	7.88724600	1.92335000
S	29.57408600	7.45122400	1.99068800
S	33.20366700	7.41181000	1.86982400
H	22.34766100	2.87431700	2.38289900
H	26.53567800	3.42173900	1.84125400
H	29.52716000	4.78908100	2.26169900
H	32.60029200	4.66960000	2.37202400

H	22.19851400	10.49667500	2.38413300
H	25.27821300	10.55191000	2.37967800
H	28.22158800	11.74173000	1.86593400
H	32.40428500	12.26590000	2.38970400
H	22.22817300	6.65440400	2.35526700
H	26.01087100	6.72595700	2.76704200
H	32.46789300	8.42266100	2.37271200
Al	27.58115800	7.86739200	2.87436000
C	27.03728900	6.10523300	3.80201400
H	26.12267200	5.88732100	4.36135400
H	27.33904700	5.21010300	3.26067400
H	27.79798800	6.29320900	4.57626900
S	27.59332700	9.55935100	4.29070100
H	26.49022200	9.11482400	4.92342900
Im1 ^{B6}			
Si	-3.85075800	5.72541600	-1.81949700
Si	-5.77077400	5.72352100	-0.46190600
Si	-3.84696400	1.88531000	-1.81941000
Si	-5.76694700	1.88318600	-0.46180900
Si	-3.84886000	3.80541700	-3.17719200
Si	-0.01086000	5.72941100	-1.81949200
Si	-1.93077600	5.72730900	-0.46190600
Si	-0.00709600	1.88921600	-1.81939000
Si	-1.92677200	1.88728700	-0.46197200
Si	-0.00875600	3.80931200	-3.17720100

Si	-3.84317100	-1.95478900	-1.81938000
Si	-5.76303500	-1.95669500	-0.46200300
Si	-3.84495800	-0.03468700	-3.17730000
Si	-3.83916000	-5.79478400	-1.81949800
Si	-5.75916200	-5.79688700	-0.46189300
Si	-3.84105800	-3.87478400	-3.17720200
Si	-0.00295800	-1.95076800	-1.81945500
Si	-1.92290900	-1.95238300	-0.46175600
Si	-0.00486600	-0.03078700	-3.17718500
Si	0.00096000	-5.79098100	-1.81943900
Si	-1.91925700	-5.79257600	-0.46198600
Si	-0.00096500	-3.87088600	-3.17718700
Si	3.82933900	5.73321100	-1.81949600
Si	1.90946100	5.73120100	-0.46199800
Si	3.83312100	1.89308900	-1.81941700
Si	1.91339800	1.89083600	-0.46206900
Si	3.83133700	3.81320700	-3.17720400
Si	5.74945300	5.73502200	-0.46190500
Si	5.75339200	1.89501800	-0.46193000
Si	3.83717100	-1.94707300	-1.81935100
Si	1.91724300	-1.94884100	-0.46213400
Si	3.83524400	-0.02689500	-3.17728800
Si	3.84116800	-5.78710900	-1.81947800
Si	1.92098300	-5.78910600	-0.46210200
Si	3.83912900	-3.86698600	-3.17720500
Si	5.75709100	-1.94459800	-0.46156900

Si	5.76081500	-5.78478800	-0.46192100
H	-3.82135800	6.92261400	-2.73079500
H	-1.91345800	6.91491300	0.45920400
H	-7.08835900	1.91792000	-1.15379500
H	-0.01115800	6.99041600	-2.63119200
H	-7.01766000	5.40471700	-1.22029600
H	-5.90005700	6.98051300	0.33280400
H	-2.98615900	3.83311300	-4.38229600
H	-5.26095900	3.81791300	-3.71489600
H	1.16254100	3.76771300	-4.07989600
H	-1.18205900	3.75971300	-4.07649600
H	-2.99385900	-0.02128700	-4.39419600
H	-5.25965900	-0.02478700	-3.71499600
H	1.16024100	-0.01528700	-4.09019600
H	-1.19255900	-0.01698700	-4.05959600
H	1.16594100	-3.81168700	-4.08559600
H	-1.17615900	-3.80718700	-4.07359600
H	3.81924000	6.92911300	-2.73229600
H	5.84843700	6.96791300	0.37810500
H	7.01834000	5.46031300	-1.19879800
H	1.90193900	6.92601300	0.44740500
H	7.08353500	1.93691000	-1.13620900
H	5.24464100	3.81961300	-3.71289600
H	2.96904100	3.84031300	-4.38189600
H	7.08415300	-1.92187900	-1.14397200
H	5.24504100	-0.01308700	-3.72639600

H	2.96914100	-0.01068700	-4.38189600
H	1.91551000	-6.98967300	0.43672200
H	3.83384100	-6.97418900	-2.74439300
H	7.02065100	-5.49249100	-1.20928000
H	5.87064600	-7.02688900	0.35820000
H	5.25184100	-3.85678700	-3.71499600
H	2.97624100	-3.87578700	-4.38199600
H	0.00493600	-7.04139300	-2.64758600
H	-5.86735800	-7.04188800	0.35380300
H	-7.01525800	-5.50808800	-1.21689800
H	-7.08256600	-1.92738700	-1.15888200
H	-3.82065900	-6.98018800	-2.74729500
H	-1.90006100	-6.98998700	0.44130400
H	-2.97885900	-3.88788700	-4.38319600
H	-5.25245900	-3.87768700	-3.71869600
Si	-5.04840800	-0.03531400	0.75809100
Si	-5.06522000	3.81358900	0.78175100
Si	-2.60832000	3.80482800	0.75495900
Si	-5.05679300	-3.88168400	0.76097200
Si	-2.57020700	-0.02842700	0.75290800
Si	-2.60158800	-3.87183600	0.76861900
Si	2.57572300	-0.02939800	0.74777300
Si	2.58504800	3.80933300	0.76674900
Si	5.03853100	3.81602000	0.76552000
Si	2.59062300	-3.86493600	0.75797900
Si	5.04756200	-0.02990300	0.75445000

Si	5.05323500	-3.87570000	0.78175300
S	-5.78244000	-3.70756100	2.79732500
S	-2.17112300	-3.92950700	2.88434000
S	1.78524800	-4.04623000	2.75930000
S	5.78156400	-4.07390000	2.79848100
S	-5.79967100	3.99992000	2.79878600
S	-1.83217500	4.02916200	2.76434300
S	2.08532100	3.83937700	2.87584200
S	5.73092100	3.63674100	2.81170300
S	-5.77251900	0.14919000	2.78493900
S	-2.02559800	0.06808800	2.85468900
S	2.06237300	-0.12532300	2.85693400
S	5.75008400	-0.20733800	2.78830600
H	-5.04303400	-4.72222300	3.28311200
H	-0.85213800	-4.18693100	2.76009600
H	1.97519900	-2.75956200	3.11487800
H	5.18670500	-2.96640200	3.28205700
H	-5.21713800	2.88166900	3.27244200
H	-2.24565700	2.83049000	3.21985700
H	0.81530400	4.26079200	2.71876100
H	4.97979000	4.64706200	3.28919100
H	-5.13105500	-0.93550300	3.26292500
H	-0.32787900	-2.16240100	4.32313700
H	5.01090500	0.80980300	3.27341400
Al	0.04900200	0.53857300	3.41799300
C	0.10011200	-2.27664300	5.32240500

H	-0.57448600	-1.83467200	6.05507200
H	0.21370800	-3.34226200	5.52495400
H	1.07519500	-1.79148100	5.38766200
S	0.09490000	1.59610200	5.32186500
H	-1.23213400	1.48622800	5.51661100
P^{B6}			
Si	23.54399900	13.33659800	-2.71529800
Si	21.62400400	13.33468300	-1.35769300
Si	23.54778300	9.49647800	-2.71517600
Si	21.62785200	9.49433900	-1.35763900
Si	23.54590100	11.41659800	-4.07300500
Si	27.38389900	13.34059700	-2.71530200
Si	25.46399800	13.33847600	-1.35769700
Si	27.38770500	9.50035700	-2.71526200
Si	25.46777000	9.49839000	-1.35775900
Si	27.38599900	11.42049700	-4.07300600
Si	23.55157900	5.65640200	-2.71516200
Si	21.63176900	5.65452600	-1.35781200
Si	23.54980000	7.57649900	-4.07309300
Si	23.55559900	1.81640500	-2.71530000
Si	21.63561000	1.81431800	-1.35770000
Si	23.55370100	3.73640100	-4.07300400
Si	27.39179200	5.66044900	-2.71525600
Si	25.47165600	5.65902100	-1.35759400
Si	27.38989800	7.58039700	-4.07299900

Si	27.39569800	1.82020300	-2.71520200
Si	25.47549900	1.81864600	-1.35779400
Si	27.39380400	3.74029800	-4.07299900
Si	31.22410100	13.34440000	-2.71529800
Si	29.30419400	13.34238200	-1.35779900
Si	31.22791600	9.50431000	-2.71517400
Si	29.30829600	9.50196900	-1.35789200
Si	31.22610100	11.42440000	-4.07300200
Si	33.14420000	13.34619400	-1.35769700
Si	33.14807400	9.50619500	-1.35769800
Si	31.23190700	5.66409900	-2.71518900
Si	29.31206600	5.66228300	-1.35804300
Si	31.22999700	7.58430000	-4.07310000
Si	31.23589900	1.82410200	-2.71530000
Si	29.31579700	1.82211400	-1.35779300
Si	31.23390100	3.74420100	-4.07300200
Si	33.15187100	5.66661900	-1.35742000
Si	33.15560100	1.82640500	-1.35769700
H	23.57339900	14.53380200	-3.62659800
H	25.48130500	14.52609700	-0.43659700
H	20.30640600	9.52908900	-2.04961100
H	27.38360000	14.60160000	-3.52700000
H	20.37710000	13.01589800	-2.11609900
H	21.49469800	14.59169800	-0.56299700
H	24.40860000	11.44430000	-5.27810000
H	22.13380000	11.42910000	-4.61070000

H	28.55730000	11.37890000	-4.97570000
H	26.21270000	11.37090000	-4.97230000
H	24.40090000	7.58990000	-5.29000000
H	22.13510000	7.58640000	-4.61080000
H	28.55500000	7.59590000	-4.98600000
H	26.20220000	7.59420000	-4.95540000
H	28.56070000	3.79950000	-4.98140000
H	26.21860000	3.80400000	-4.96940000
H	31.21400000	14.54030100	-3.62809900
H	33.24320100	14.57909900	-0.51769900
H	34.41310000	13.07150000	-2.09460000
H	29.29669700	14.53719800	-0.44839800
H	34.47829600	9.54809400	-2.03200800
H	32.63940000	11.43080000	-4.60870000
H	30.36380000	11.45150000	-5.27770000
H	34.47889800	5.68930400	-2.03980300
H	32.63980000	7.59810000	-4.62220000
H	30.36390000	7.60050000	-5.27770000
H	29.31029800	0.62150200	-0.45909800
H	31.22860000	0.63699900	-3.64019900
H	34.41540000	2.11870000	-2.10510000
H	33.26540100	0.58430100	-0.53759900
H	32.64660000	3.75440000	-4.61080000
H	30.37100000	3.73540000	-5.27780000
H	27.39970000	0.56979900	-3.54339900
H	21.52740000	0.56930100	-0.54199800

H	20.37949900	2.10310200	-2.11269800
H	20.31220200	5.68380900	-2.05470300
H	23.57409900	0.63099800	-3.64309800
H	25.49470800	0.62120400	-0.45449500
H	24.41590000	3.72330000	-5.27900000
H	22.14230000	3.73350000	-4.61450000
Si	22.34591600	7.57580000	-0.13861800
Si	22.32888800	11.42469300	-0.11363500
Si	24.78589800	11.41549900	-0.14032000
Si	22.33996200	3.72926300	-0.13405900
Si	24.82365100	7.58267600	-0.14508400
Si	24.79617300	3.74009400	-0.12432400
Si	29.97045200	7.58168700	-0.14661800
Si	29.97897900	11.42074100	-0.12936700
Si	32.43256500	11.42738500	-0.13087800
Si	29.98597700	3.74599600	-0.13789100
Si	32.44253800	7.58104300	-0.14180500
Si	32.44832200	3.73542200	-0.11441300
S	21.61369900	3.90375500	1.90208000
S	25.23653300	3.68596500	1.98934100
S	29.18838600	3.55968000	1.86608900
S	33.17812900	3.53483800	1.90158700
S	21.59355500	11.61211500	1.90289800
S	25.56171700	11.63818700	1.87040200
S	29.47412400	11.45616100	1.97953800
S	33.12614400	11.24780700	1.91547300

S	21.62101300	7.76216400	1.88770700
S	25.37108400	7.68458200	1.95522700
S	29.45454100	7.49776000	1.96396400
S	33.16133700	7.39009800	1.88390900
H	22.35728200	2.89265200	2.38907900
H	26.55838800	3.45079100	1.85474500
H	29.37752800	4.84670400	2.21896200
H	32.58272300	4.64009000	2.38948400
H	22.17343800	10.49266000	2.37688300
H	25.13644500	10.44505000	2.33026600
H	28.21467100	11.90703400	1.82046400
H	32.36527100	12.24812900	2.39862400
H	22.25908700	6.67569200	2.36623700
H	32.51381000	8.46847000	2.36738900
Al	27.44177900	8.16881900	2.51120900
S	27.48066900	9.13506200	4.46094900
H	26.15002000	9.04306000	4.63708800