

TSA in gas phase

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

C H

7 15

direct

| | | |
|----------------|----------------|----------------|
| 0.797168190522 | 0.590274923733 | 0.605993333470 |
| 0.712109079831 | 0.815287482659 | 0.520182423771 |
| 0.691905517916 | 0.702146296130 | 0.620384589513 |
| 0.551931422123 | 0.687287906738 | 0.623889210077 |
| 0.604273111951 | 0.595279768548 | 0.843018617880 |
| 0.600441871031 | 0.704573777539 | 0.732882444479 |
| 0.515423663291 | 0.820551657665 | 0.761596139827 |
| 0.833914711891 | 0.589830690060 | 0.510886211989 |
| 0.868926330950 | 0.594604533645 | 0.630723431828 |
| 0.775769085780 | 0.505030290217 | 0.663836872741 |
| 0.741679366001 | 0.800396682499 | 0.431408184128 |
| 0.787319210583 | 0.832743606613 | 0.526781130619 |
| 0.606367134503 | 0.629033848738 | 0.563902060502 |
| 0.660297014010 | 0.598355409108 | 0.888592064883 |
| 0.644275580255 | 0.508451872454 | 0.822482192923 |
| 0.633591766991 | 0.896026076947 | 0.524534433268 |
| 0.502296103024 | 0.777333101956 | 0.578319320327 |
| 0.491476197152 | 0.637875615437 | 0.701271403580 |
| 0.512930103700 | 0.599459221915 | 0.906890057341 |
| 0.552824623362 | 0.839694318917 | 0.814317751551 |
| 0.504635283691 | 0.899182288417 | 0.681998319454 |
| 0.426024831429 | 0.808673580112 | 0.819919195893 |

TSB in gas phase

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

C H

7 15

Cartesian

| | | |
|-------------------|-------------------|---------------|
| -2.25543491264 | 0.513351237895 | 12.0246966741 |
| -0.94195129735 | -0.551605634526 | 13.9136624957 |
| -0.88973316431 | 0.271374841546 | 12.6400273618 |
| -0.589723088364 | 2.85894828584 | 12.1437071053 |
| 0.0668333190604 | 1.61089809034 | 12.729337998 |
| 0.246183666399 | 0.116996166619 | 11.763644998 |
| 0.759204603372 | 1.76701026652 | 14.0812902948 |
| -2.87708770865 | 1.12629122693 | 12.6933569275 |
| -2.75417155932 | -0.459569079894 | 11.9054228361 |
| -2.2062546032 | 0.998137274813 | 11.0416621533 |
| -1.49905858817 | -1.47569532566 | 13.700881349 |
| -1.49580726189 | 3.09314392199 | 12.7200814772 |
| -1.48491970834 | -0.00920605129108 | 14.7012322012 |
| -0.869543574334 | 2.73371165765 | 11.0904616157 |
| -0.00295401746961 | 1.88080904131 | 14.8649796625 |
| 0.0509191465031 | -0.826873905445 | 14.2908425963 |
| 0.111187099178 | 3.70138320213 | 12.2238230476 |
| 0.144849519302 | 0.320055670715 | 10.6915470629 |
| 0.980000910242 | 1.46932553535 | 12.0139778362 |

1.11559489317 -0.466017245607 12.0879556893
1.38472025128 2.67009775726 14.0586711406
1.39242310462 0.907392479361 14.3332643348

Reactant R(I) in gas phase

1.0

-7.923687999980 -0.000017000000 9.876321999989
3.961560999998 -6.862258999981 9.876106000012
3.961547000001 6.862197999978 9.876069999981

C H

7 15

Cartesian

-1.63397216941 -1.37003587931 13.0558480191
-1.10458369863 0.729544535945 11.7795396016
-0.937563110463 -0.688778444393 11.9639422744
-0.0274692153723 -1.45691259604 11.1159987572
0.043834215743 1.25725261833 14.0860708676
0.0914361365063 1.50325573747 12.5867010711
1.46488525278 1.26435489878 11.9828994954
-2.63900691631 -1.61752719547 12.6429457579
-2.03789867614 1.10241925803 12.2237740076
-1.83165263741 -0.699606814727 13.9059503255
-1.16778884431 -2.31787338964 13.3582081487
-0.984350917332 1.03434991958 10.7310387038
-0.964484168836 1.40891409589 14.5014980606
-0.434926498484 -2.46190512369 10.9077372715
-0.216453632331 2.54106281096 12.3788003514
0.283633737695 -0.939113543656 10.2021363014
0.393465776949 0.24760332825 14.3537029287
0.715287240476 1.97597957381 14.5807622997
0.873363547859 -1.66108295524 11.7379381473
1.47205117583 1.41204671089 10.8927895906
1.85723631682 0.261479708688 12.2126788101
2.16813594123 1.98764856532 12.4244205672

Reactant R(II) in gas phase

1.0

-7.923687999980 -0.000017000000 9.876321999989
3.961560999998 -6.862258999981 9.876106000012
3.961547000001 6.862197999978 9.876069999981

H C

15 7

Cartesian

0.722430910038 2.47755828551 20.6767787734
0.348550388689 -2.65288759499 20.3571714898
-1.20637940988 -3.42786066157 20.9385193515
-0.790702244299 -3.31798224426 19.2041709793
-1.14561437361 0.870516789881 21.0863266087
0.206358956013 -0.720153429493 18.8165067205
-1.36583289726 0.20912593016 18.7339223438
1.32530768063 1.46747788034 19.3368620365
1.11031932235 0.599823861132 22.2423301406
1.58787609632 -0.562384765669 20.989572611
0.241240445631 -0.942005823533 22.1062550704
-2.7567481725 -1.39568162284 21.5512953349
-3.39342106701 -2.20746098553 20.1520868442
-3.24818484005 -0.39424446287 20.1281921516
-0.266781319495 2.27545365737 19.203259712

-0.730914676986 -2.78879822884 20.1828458542
-0.703372343964 -0.414388378919 19.3515686564
-1.40732596251 -1.51044210284 19.9649922282
-0.227707066622 0.558493030261 20.5634795484
0.422340157289 1.7655088957 19.891464812
0.722093750492 -0.139903748004 21.5260772143
-2.77958635163 -1.33403831216 20.4424362693

Reactant R(III) in gas phase

1.0

-7.923687999980 -0.000017000000 9.876321999989
3.961560999998 -6.862258999981 9.876106000012
3.961547000001 6.862197999978 9.876069999981

C H

7 15

Cartesian

-2.22462252358 -0.95333006729 14.4032950905
-1.70396097037 2.61906513794 14.3525717265
-1.22465819502 -0.280125531615 13.4692203249
-0.596811118942 1.84263513226 13.772659941
-0.407080192673 -1.23277229809 12.6035878382
-0.18940731956 0.606827660697 14.3769856598
0.0963296531514 2.34242018717 12.5750471692
-2.94265628155 -1.53228400784 13.802847063
-2.79464251581 -0.223380162189 14.997831123
-2.35027381132 2.01334506231 15.003285829
-2.27816799345 3.18293261415 13.6048098169
-1.80361958494 0.373878256828 12.7831749277
-1.70203868605 -1.6337049998 15.0920348974
-1.21654015581 3.36796858098 15.0143724189
-1.09100194656 -1.81819741006 11.9704544786
-0.553720922087 2.92286277395 11.9063565782
-0.454123602079 0.492872865344 15.4338706061
0.171624294535 -1.92059129661 13.2379285387
0.290237358481 -0.697925482496 11.941064677
0.64287523421 1.55180104802 12.0417789488
0.837021905653 0.293743046132 14.1566697976
0.869248518799 3.04314878853 12.9601377751

Product P in gas phase

1.0

-7.923687999980 -0.000017000000 9.876321999989
3.961560999998 -6.862258999981 9.876106000012
3.961547000001 6.862197999978 9.876069999981

C H

7 15

Cartesian

-2.33518207553 -0.362024045177 11.1900585425
-1.68724447183 2.24609691664 12.2842132519
-0.964892311314 -0.0929981309279 11.6413694714
-0.792056008697 0.451368619284 13.8511122407
-0.658039362265 1.11830074808 12.3994552483
0.0688529894739 -1.07646227456 11.3084543885
0.773160819843 1.65379304433 12.2470073886
-3.07480481686 -0.0988850624292 11.9642055133
-2.7048622629 1.9261120063 12.5479936325
-2.54546160744 0.363998888339 10.3754290776
-2.48766803579 -1.38317157079 10.8227816587

-1.80474071793 0.0742874636864 14.0473774255
-1.69960711773 2.65397065236 11.2618574982
-1.40260981763 3.05475722075 12.9713852063
-0.585740265886 1.29536580969 14.5283456784
-0.319020357944 -2.10603055473 11.3206278167
-0.0459450406625 -0.336191353259 14.0193667703
0.313871264803 -0.869225862366 10.2407068891
0.897716916364 2.4991238964 12.9381812581
0.939477778571 2.01834622621 11.222542237
1.00168107789 -0.972069257933 11.8730189258
1.54322705375 0.90966334408 12.4895975551

Type B isomerisation, configuration R1 of the reactant

1
-7.923688 -0.000017 9.876322
3.961561 -6.862259 9.876106
3.961547 6.862198 9.876070
Si Al O H C
23 1 48 15 7
Direct configuration= 1117
0.12356296 0.74097710 0.29055458
0.62468632 0.23567326 0.79174907
0.85476383 0.46526922 0.32326736
0.34904873 0.96976966 0.83852298
0.89578274 0.19526914 0.05742711
0.40561491 0.68843159 0.56366688
0.74833597 0.36142125 0.22321871
0.24956594 0.86015969 0.72292490
0.01814559 0.63424545 0.18416410
0.51661700 0.13498947 0.68252796
0.29257015 0.59269393 0.45813460
0.79415268 0.08258599 0.95022319
0.28708087 0.36363790 0.68866161
0.78774291 0.86360518 0.18546518
0.73912485 0.13988918 0.45267485
0.24445426 0.63663833 0.95215328
0.39466946 0.46165759 0.79608250
0.89525153 0.97020047 0.28953752
0.12304075 0.19528257 0.83545142
0.62106068 0.70001399 0.32524636
0.35038467 0.74271018 0.06048646
0.84770803 0.24732809 0.55886136
0.51609366 0.59550833 0.22801347
0.02193900 0.08493105 0.71739507
0.23184967 0.78177501 0.17085890
0.73096710 0.28020199 0.67345638
0.23579358 0.08151093 0.88172439
0.73546010 0.57969370 0.33530011
0.93440772 0.08016780 0.17141644
0.43554343 0.56553425 0.67297051
0.69998900 0.25545263 0.34028029
0.20819911 0.74685145 0.83788278
0.40785810 0.25677238 0.64741819
0.90478568 0.75013066 0.15156294
0.41213737 0.54954139 0.35018736
0.90320769 0.04103045 0.84099978
0.17501087 0.66692747 0.40722932
0.66831244 0.16151271 0.91262867

| | | |
|------------|------------|------------|
| 0.46789329 | 0.01676307 | 0.75602707 |
| 0.97598805 | 0.51099502 | 0.25531544 |
| 0.81123295 | 0.31505348 | 0.10373761 |
| 0.34796679 | 0.80607866 | 0.61084346 |
| 0.46649284 | 0.65708463 | 0.11063697 |
| 0.97290687 | 0.17461513 | 0.58929046 |
| 0.16909570 | 0.31618782 | 0.75956486 |
| 0.66633842 | 0.81991397 | 0.26310848 |
| 0.82068119 | 0.01957576 | 0.40733457 |
| 0.32298538 | 0.51178176 | 0.91422729 |
| 0.01813337 | 0.86404056 | 0.31490746 |
| 0.51398881 | 0.35341709 | 0.82286900 |
| 0.86082547 | 0.37614783 | 0.45609967 |
| 0.37946476 | 0.86596387 | 0.96099276 |
| 0.02036641 | 0.22288384 | 0.96015386 |
| 0.53226516 | 0.70077694 | 0.46004162 |
| 0.63380775 | 0.48084607 | 0.20450139 |
| 0.13714002 | 0.95966111 | 0.68018269 |
| 0.12322414 | 0.61187995 | 0.06084968 |
| 0.61774813 | 0.11240313 | 0.55724210 |
| 0.26579955 | 0.47350531 | 0.56721686 |
| 0.76236030 | 0.96618099 | 0.06394501 |
| 0.07158129 | 0.65537921 | 0.26901691 |
| 0.57430665 | 0.15127611 | 0.76630614 |
| 0.85082669 | 0.39325353 | 0.24347340 |
| 0.32044385 | 0.91268348 | 0.76413877 |
| 0.82002730 | 0.16612257 | 0.00233558 |
| 0.31505999 | 0.68056673 | 0.50653392 |
| 0.07641319 | 0.16564453 | 0.75585283 |
| 0.55092100 | 0.69810398 | 0.24322364 |
| 0.30452178 | 0.41043281 | 0.78117122 |
| 0.81197258 | 0.91616041 | 0.26847582 |
| 0.32545208 | 0.66544787 | 0.00286341 |
| 0.81886114 | 0.17016801 | 0.50232708 |
| 0.42375624 | 0.11071755 | 0.21832709 |
| 0.35779935 | 0.07786210 | 0.08477500 |
| 0.27791068 | 0.96744161 | 0.20071974 |
| 0.22733546 | 0.06995315 | 0.07347703 |
| 0.28293130 | 0.38253325 | 0.15538495 |
| 0.24305407 | 0.29536039 | 0.05031342 |
| 0.11145040 | 0.34373088 | 0.17026572 |
| 0.45316196 | 0.21921416 | 0.07206873 |
| 0.24288105 | 0.17677113 | 0.39448610 |
| 0.13594073 | 0.32376364 | 0.36532040 |
| 0.28210528 | 0.30666365 | 0.36630347 |
| 0.09868540 | 0.13962694 | 0.38470840 |
| 0.08245486 | 0.03266962 | 0.33706721 |
| 0.00075673 | 0.19390023 | 0.29901701 |
| 0.47234567 | 0.23297399 | 0.19622044 |
| 0.26995305 | 0.06048440 | 0.14017157 |
| 0.19837564 | 0.27466937 | 0.14866690 |
| 0.18531568 | 0.15340487 | 0.19942967 |
| 0.28511926 | 0.28708601 | 0.20442415 |
| 0.41523501 | 0.20748828 | 0.17016321 |
| 0.23234886 | 0.27241955 | 0.33997225 |
| 0.08772014 | 0.12504732 | 0.30910745 |

Type B isomerization, configuration TS1 of the TS

1.0000000000000000
-7.9236880000000003 -0.0000170000000000 9.8763220000000000
3.9615610000000001 -6.8622589999999999 9.8761060000000001
3.9615469999999999 6.8621980000000002 9.8760700000000003

Si Al O H C
23 1 48 15 7

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1231177167538590 | 0.7384552130632331 | 0.2922083865486318 |
| 0.6244884416689330 | 0.2369529717654269 | 0.7933861242806615 |
| 0.8520723269217302 | 0.4665600125795520 | 0.3249781589784012 |
| 0.3530538357640307 | 0.9657877418217468 | 0.8403543325110129 |
| 0.8990721792624751 | 0.1908714166886112 | 0.0619906868462452 |
| 0.4019794383489370 | 0.6912304755953635 | 0.5618906475279849 |
| 0.7480488364574026 | 0.3582437771405653 | 0.2270695535340586 |
| 0.2498465939943692 | 0.8613238184914984 | 0.7244103472328030 |
| 0.0172629828275608 | 0.6345193024522372 | 0.1822856603167185 |
| 0.5171859413386697 | 0.1332203551925565 | 0.6888975853939203 |
| 0.2909697055908702 | 0.5895495776854288 | 0.4611439557816183 |
| 0.7963969586920434 | 0.0841305138009650 | 0.9505130791807379 |
| 0.2891645730868886 | 0.3602292727164838 | 0.6920268740408564 |
| 0.7872963757910882 | 0.8630911379600970 | 0.1854301738671751 |
| 0.7451713112954227 | 0.1356517227177733 | 0.4571700077383232 |
| 0.2425054402002096 | 0.6377607460216123 | 0.9520260493007275 |
| 0.3986250089542584 | 0.4640139718982864 | 0.7934606232921326 |
| 0.8927042114938324 | 0.9642447471036528 | 0.2953826799367991 |
| 0.1251090824851590 | 0.1925953064098840 | 0.8430073099822848 |
| 0.6193369269899035 | 0.6999719498703801 | 0.3240110536628246 |
| 0.3486032438361647 | 0.7413271064204235 | 0.0638617069745142 |
| 0.8513203719728069 | 0.2445824850557304 | 0.5586929984210953 |
| 0.5151003294695528 | 0.5900874908431454 | 0.2305569938617791 |
| 0.0218647153096331 | 0.0879578191770999 | 0.7218186976331079 |
| 0.2307118511773808 | 0.7823031777507266 | 0.1736690493627175 |
| 0.7282457870340373 | 0.2752863300517612 | 0.6693014682476289 |
| 0.2398670659117100 | 0.0776698940172939 | 0.8814621265534689 |
| 0.7326432588330046 | 0.5797780571640520 | 0.3428755476911896 |
| 0.9314528380189020 | 0.0732422618031972 | 0.1762460318506031 |
| 0.4363718420778208 | 0.5678397203427702 | 0.6695126839112644 |
| 0.7034240447154640 | 0.2526550793623436 | 0.3468880236809570 |
| 0.2050026565835071 | 0.7490737511109409 | 0.8391833879502685 |
| 0.4077455146445702 | 0.2524150191673865 | 0.6494324974574123 |
| 0.9056434407534001 | 0.7515955479642749 | 0.1476789355746426 |
| 0.4123271600311395 | 0.5459753481040895 | 0.3550113266775423 |
| 0.9038154744738208 | 0.0386652352543894 | 0.8424728230475196 |
| 0.1744535799300709 | 0.6595715235745963 | 0.4087004888640993 |
| 0.6710849086507765 | 0.1659633848425733 | 0.9124798878347122 |
| 0.4722802327743165 | 0.0125481223403293 | 0.7582180148446368 |
| 0.9732646791046156 | 0.5124965090994347 | 0.2547056228301979 |
| 0.8131267620653422 | 0.3098302747324626 | 0.1090314897670264 |
| 0.3439139806460595 | 0.8072027149607560 | 0.6112866883586693 |
| 0.4631122193087985 | 0.6505685270467707 | 0.1149272877738138 |
| 0.9730989508936628 | 0.1815204934177914 | 0.5950509994809071 |
| 0.1705435336315177 | 0.3143176046738355 | 0.7688055763324420 |
| 0.6659034253857921 | 0.8190629218183999 | 0.2576367022435832 |
| 0.8168999398903816 | 0.0144114493380267 | 0.4124615832309816 |
| 0.3235506783473635 | 0.5143327681239297 | 0.9115918320210417 |
| 0.0153447707151200 | 0.8581867836005511 | 0.3209237795544888 |
| 0.5195400130110398 | 0.3596013275457832 | 0.8211811236241684 |
| 0.8614163067668106 | 0.3741233191112595 | 0.4554878662185538 |

| | | |
|--------------------|--------------------|---------------------|
| 0.3824554117708981 | 0.8618601420711116 | 0.9632847874752835 |
| 0.0263919771620952 | 0.2174105361915766 | 0.97081111798643362 |
| 0.5258381322486601 | 0.7077651673890806 | 0.4554733430919628 |
| 0.6305461112346783 | 0.4737064067244041 | 0.2073794228647857 |
| 0.1392109357590611 | 0.9651133839630026 | 0.6826015650867500 |
| 0.1226011289490721 | 0.6063045263211642 | 0.0601681870823326 |
| 0.6250089258637079 | 0.1128182270184920 | 0.5667884868122167 |
| 0.2654133808298874 | 0.4705651284154404 | 0.5717739598422561 |
| 0.7618552919434076 | 0.9704496032174466 | 0.0665343267463979 |
| 0.0734404691888051 | 0.6543024816312347 | 0.2653378494418768 |
| 0.5634552937766861 | 0.1538194054030247 | 0.7794866546884586 |
| 0.8477450251342462 | 0.3987764163902043 | 0.2417761053009645 |
| 0.3265761177942119 | 0.9069761632859746 | 0.7656579574531283 |
| 0.8265426312188494 | 0.1674715519125720 | 0.9988475606675578 |
| 0.3101913814014389 | 0.6803519472484356 | 0.5086003953750559 |
| 0.0714714913180658 | 0.1685491112815387 | 0.7654034157102891 |
| 0.5541950311525980 | 0.6922279635233894 | 0.2411288939586574 |
| 0.3112607718270963 | 0.4064727236433331 | 0.7823483345323804 |
| 0.8098220453559931 | 0.9088578946836997 | 0.2750221782037461 |
| 0.3199091065039666 | 0.6663238042626690 | 0.0065442232637283 |
| 0.8343926089061285 | 0.1612056088710198 | 0.4994927791028096 |
| 0.4368243653989881 | 0.1723365296127237 | 0.1791918289458729 |
| 0.3720287232507193 | 0.1402963298650939 | 0.0169434985986455 |
| 0.3724042493706895 | 0.0272776260876600 | 0.1598431304920248 |
| 0.2766831044527059 | 0.0452938328746990 | 0.0791023512089062 |
| 0.2054276569915876 | 0.3742612361966380 | 0.1389481557887237 |
| 0.2074345026739643 | 0.3375252035495742 | 0.0031837186655854 |
| 0.0659393910546289 | 0.3524327345409897 | 0.1338034391541441 |
| 0.4165655281999193 | 0.2789205820173575 | 0.0385098309382062 |
| 0.2351926214011419 | 0.1900581683033464 | 0.3813164639831870 |
| 0.0977297135570921 | 0.2992633414910759 | 0.3566317051767499 |
| 0.2212933448430718 | 0.3483650476009295 | 0.3311557656750730 |
| 0.1681490188188456 | 0.0577369232493773 | 0.3499845075429904 |
| 0.0994144429480017 | 0.0629258832066060 | 0.2497038620281906 |
| 0.0410582141503976 | 0.1820937371873118 | 0.3167589613695118 |
| 0.4042716008530890 | 0.3307749957315008 | 0.1547668068481770 |
| 0.3149267732040523 | 0.0942536530182779 | 0.1015903391354938 |
| 0.1608267936762394 | 0.3026682725076077 | 0.0992675565050025 |
| 0.2106435148727766 | 0.1806188726735674 | 0.1682147369860994 |
| 0.2501519676300443 | 0.2752446889258002 | 0.1919472491805408 |
| 0.3851703787700800 | 0.2637114827184047 | 0.1366602761041872 |
| 0.1964474554845169 | 0.2789973643398243 | 0.3231679977167362 |
| 0.1244500554898912 | 0.1182259844606044 | 0.2782221332837815 |

Type B isomerisation, configuration P1 of the product

| | | |
|-----------|-----------|----------|
| 1 | | |
| -7.923688 | -0.000017 | 9.876322 |
| 3.961561 | -6.862259 | 9.876106 |
| 3.961547 | 6.862198 | 9.876070 |
| Si | Al | O |
| 23 | 1 | 48 |
| | H | C |
| | 15 | 7 |

Direct configuration= 1188

| | | |
|------------|------------|------------|
| 0.12437766 | 0.74054442 | 0.28990449 |
| 0.62265232 | 0.23518165 | 0.79386318 |
| 0.85283090 | 0.46693141 | 0.32489883 |
| 0.34987821 | 0.96838991 | 0.83781582 |
| 0.89515881 | 0.19460888 | 0.05854533 |
| 0.40544890 | 0.68812708 | 0.56459163 |

| | | |
|------------|------------|------------|
| 0.74862389 | 0.36104000 | 0.22453408 |
| 0.24806041 | 0.86111639 | 0.72244365 |
| 0.01805883 | 0.63400476 | 0.18505861 |
| 0.51652795 | 0.13394632 | 0.68330625 |
| 0.29208973 | 0.58994883 | 0.45882106 |
| 0.79312723 | 0.08444057 | 0.95125580 |
| 0.28763123 | 0.36316517 | 0.68691791 |
| 0.78603313 | 0.86438359 | 0.18773670 |
| 0.74146525 | 0.13922570 | 0.45403440 |
| 0.24194882 | 0.63704290 | 0.95211110 |
| 0.39610911 | 0.46395293 | 0.79441958 |
| 0.89337388 | 0.96888806 | 0.29151941 |
| 0.12479008 | 0.19392555 | 0.83690528 |
| 0.61960923 | 0.70154480 | 0.32390769 |
| 0.34961955 | 0.74187892 | 0.06034807 |
| 0.84675168 | 0.24845215 | 0.56045818 |
| 0.51569971 | 0.59398380 | 0.22763957 |
| 0.02154572 | 0.08734695 | 0.71852514 |
| 0.23162668 | 0.78266501 | 0.17007057 |
| 0.72867652 | 0.27947208 | 0.67519882 |
| 0.23727535 | 0.07965273 | 0.88137917 |
| 0.73550940 | 0.58322140 | 0.33648056 |
| 0.93174820 | 0.07752451 | 0.17159379 |
| 0.44162920 | 0.56841161 | 0.67461661 |
| 0.70131114 | 0.25480714 | 0.34201851 |
| 0.20700723 | 0.74767047 | 0.83750039 |
| 0.40748096 | 0.25496139 | 0.64690919 |
| 0.90353478 | 0.75016880 | 0.15653068 |
| 0.41203108 | 0.54850193 | 0.35040033 |
| 0.90253624 | 0.04410898 | 0.84178728 |
| 0.17560223 | 0.66785788 | 0.40681377 |
| 0.66607506 | 0.16052753 | 0.91505087 |
| 0.46908846 | 0.01498133 | 0.75495021 |
| 0.97609975 | 0.51018617 | 0.25767425 |
| 0.81321524 | 0.31430755 | 0.10533708 |
| 0.34412089 | 0.80765424 | 0.60918575 |
| 0.46541152 | 0.65469220 | 0.11083466 |
| 0.97184523 | 0.17977816 | 0.59145848 |
| 0.17014786 | 0.31560140 | 0.76486586 |
| 0.66314217 | 0.82262417 | 0.26023781 |
| 0.82190286 | 0.01880039 | 0.40896420 |
| 0.32045259 | 0.51226351 | 0.91367998 |
| 0.01555923 | 0.86099148 | 0.31475032 |
| 0.51220237 | 0.35297094 | 0.82633012 |
| 0.85748059 | 0.37822589 | 0.45818374 |
| 0.38140619 | 0.86288462 | 0.95890367 |
| 0.02044249 | 0.22012314 | 0.96134839 |
| 0.52916473 | 0.70427183 | 0.45761595 |
| 0.63243002 | 0.47844358 | 0.20473158 |
| 0.13530678 | 0.96157183 | 0.68088775 |
| 0.11961119 | 0.61291244 | 0.05958660 |
| 0.61983892 | 0.11226151 | 0.55881164 |
| 0.26354155 | 0.46887973 | 0.56377157 |
| 0.76439759 | 0.96707228 | 0.06500619 |
| 0.07638116 | 0.65145730 | 0.26808296 |
| 0.57077559 | 0.15167379 | 0.76915259 |
| 0.84818781 | 0.39711204 | 0.24415037 |
| 0.32104397 | 0.91237147 | 0.76234760 |

| | | |
|------------|------------|------------|
| 0.81630365 | 0.17052737 | 0.00244828 |
| 0.31527780 | 0.67207714 | 0.51332999 |
| 0.07875680 | 0.16769650 | 0.75420425 |
| 0.55197725 | 0.69615589 | 0.24176541 |
| 0.30830496 | 0.41674404 | 0.77154165 |
| 0.80582523 | 0.91660995 | 0.27399247 |
| 0.32251220 | 0.66406051 | 0.00481524 |
| 0.82141902 | 0.16927847 | 0.50355944 |
| 0.45594781 | 0.17640168 | 0.21307356 |
| 0.40180940 | 0.12066254 | 0.04976156 |
| 0.38341890 | 0.99934212 | 0.18667469 |
| 0.29507251 | 0.04431620 | 0.08761339 |
| 0.09534018 | 0.34449193 | 0.14457357 |
| 0.23789327 | 0.32590153 | 0.02805066 |
| 0.13836140 | 0.24148769 | 0.06078979 |
| 0.41941312 | 0.26489493 | 0.07607892 |
| 0.15145074 | 0.20093971 | 0.42248457 |
| 0.12206803 | 0.34613111 | 0.32176293 |
| 0.24619824 | 0.29771358 | 0.37923185 |
| 0.16864303 | 0.03112826 | 0.36318831 |
| 0.10688764 | 0.06656276 | 0.24456271 |
| 0.05325384 | 0.16956351 | 0.32999495 |
| 0.38900491 | 0.33487128 | 0.18977795 |
| 0.33532317 | 0.07749553 | 0.12536687 |
| 0.17213692 | 0.27973859 | 0.10021729 |
| 0.23221938 | 0.16474486 | 0.19514492 |
| 0.27281515 | 0.22715157 | 0.23988982 |
| 0.38807371 | 0.25671719 | 0.17313385 |
| 0.19814277 | 0.26622393 | 0.34844109 |
| 0.13428249 | 0.10477739 | 0.28949448 |

Type B isomerisation, configuration R2 of the reactant

| | | | | |
|-----------|-----------|----------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |

Direct configuration= 1030

| | | |
|------------|------------|------------|
| 0.12043940 | 0.74530808 | 0.27880601 |
| 0.62279005 | 0.23962029 | 0.77626827 |
| 0.85605387 | 0.46661164 | 0.31494317 |
| 0.34541991 | 0.97415871 | 0.82352420 |
| 0.88685381 | 0.19967518 | 0.04547117 |
| 0.40500215 | 0.68996537 | 0.55527033 |
| 0.74636943 | 0.36707261 | 0.20831208 |
| 0.24732155 | 0.86066150 | 0.71353601 |
| 0.01786873 | 0.63620055 | 0.17573905 |
| 0.51244763 | 0.13961235 | 0.66623344 |
| 0.29161739 | 0.59397057 | 0.44511709 |
| 0.78738741 | 0.08794226 | 0.94675915 |
| 0.28306380 | 0.36928745 | 0.67434296 |
| 0.78712060 | 0.86545910 | 0.17348975 |
| 0.73322682 | 0.14529429 | 0.43621944 |
| 0.24782401 | 0.63569188 | 0.94370018 |
| 0.39447397 | 0.46524286 | 0.78529673 |
| 0.89412484 | 0.97596575 | 0.27441098 |
| 0.12022507 | 0.20135502 | 0.81350536 |

| | | |
|------------|------------|------------|
| 0.62359563 | 0.69890982 | 0.32038296 |
| 0.34897317 | 0.74692950 | 0.04724926 |
| 0.84316361 | 0.24821378 | 0.54737893 |
| 0.51576705 | 0.59841743 | 0.21583319 |
| 0.02014645 | 0.08878166 | 0.70904317 |
| 0.22629766 | 0.78213569 | 0.15518982 |
| 0.72642775 | 0.28997033 | 0.65823704 |
| 0.22900032 | 0.08562240 | 0.86154847 |
| 0.73755748 | 0.57984713 | 0.34012655 |
| 0.93335454 | 0.08554923 | 0.15584306 |
| 0.43838677 | 0.57290418 | 0.66791840 |
| 0.69622368 | 0.25922066 | 0.32178171 |
| 0.21196414 | 0.74627751 | 0.82914147 |
| 0.40013387 | 0.25902998 | 0.63282192 |
| 0.90528336 | 0.75243633 | 0.14110054 |
| 0.41009209 | 0.55102173 | 0.33599752 |
| 0.91271601 | 0.05503548 | 0.84695340 |
| 0.17520818 | 0.67500646 | 0.39374597 |
| 0.67112244 | 0.15766599 | 0.89328102 |
| 0.46482439 | 0.02122853 | 0.74319326 |
| 0.97660679 | 0.51277890 | 0.24283621 |
| 0.81825571 | 0.32293719 | 0.08750570 |
| 0.33836430 | 0.81192316 | 0.59626588 |
| 0.46467091 | 0.67079517 | 0.09960092 |
| 0.96239918 | 0.16487851 | 0.58656533 |
| 0.16393581 | 0.32390460 | 0.75288534 |
| 0.66708105 | 0.81998783 | 0.25407919 |
| 0.81709807 | 0.02458083 | 0.39283801 |
| 0.31954859 | 0.51044028 | 0.90598447 |
| 0.01510566 | 0.86836150 | 0.30162546 |
| 0.51167952 | 0.35418873 | 0.81318370 |
| 0.87251781 | 0.37097436 | 0.44329077 |
| 0.37325245 | 0.87127308 | 0.94658174 |
| 0.00395319 | 0.22084035 | 0.93099941 |
| 0.52995757 | 0.70736270 | 0.45170683 |
| 0.62888771 | 0.48247541 | 0.18668861 |
| 0.13024519 | 0.95890599 | 0.67864742 |
| 0.12601804 | 0.61750914 | 0.05358634 |
| 0.60864671 | 0.11917554 | 0.53759193 |
| 0.26007654 | 0.47332116 | 0.54953799 |
| 0.75856551 | 0.96529218 | 0.05144424 |
| 0.06643687 | 0.65500526 | 0.26649673 |
| 0.57350051 | 0.15928152 | 0.74403990 |
| 0.83991362 | 0.40343616 | 0.23576040 |
| 0.32355346 | 0.91580152 | 0.74491648 |
| 0.78927228 | 0.17414158 | 0.01367513 |
| 0.31931912 | 0.67152519 | 0.50053335 |
| 0.09072252 | 0.18216274 | 0.71188023 |
| 0.55763511 | 0.69056028 | 0.23873655 |
| 0.30780016 | 0.42138480 | 0.75657356 |
| 0.80983123 | 0.92321209 | 0.25282935 |
| 0.33507051 | 0.66171487 | 0.98956156 |
| 0.80623923 | 0.17825301 | 0.49070551 |
| 0.38128428 | 0.24045087 | 0.14704818 |
| 0.47002447 | 0.22240187 | 0.29488135 |
| 0.37791720 | 0.37162995 | 0.31682066 |
| 0.42465893 | 0.24816742 | 0.43611471 |
| 0.29780571 | 0.01246559 | 0.31037167 |

| | | |
|------------|------------|------------|
| 0.38663248 | 0.05025802 | 0.41771482 |
| 0.22396389 | 0.07814956 | 0.48355827 |
| 0.47947921 | 0.09058711 | 0.19065408 |
| 0.14861833 | 0.28080354 | 0.24084524 |
| 0.08947492 | 0.16019536 | 0.35421189 |
| 0.15278068 | 0.16098186 | 0.19932904 |
| 0.14681703 | 0.27117238 | 0.55078237 |
| 0.09405593 | 0.29889827 | 0.43529463 |
| 0.16290502 | 0.40786707 | 0.42375688 |
| 0.38731717 | 0.12333228 | 0.10050755 |
| 0.39464383 | 0.27303880 | 0.35546806 |
| 0.29714004 | 0.11243747 | 0.40881790 |
| 0.28540891 | 0.23436166 | 0.40246420 |
| 0.28702448 | 0.10946219 | 0.28848182 |
| 0.38981685 | 0.14314641 | 0.17618180 |
| 0.16207672 | 0.18243079 | 0.27040272 |
| 0.16826626 | 0.31254634 | 0.44785317 |

Type B isomerisation, configuration TS2 of the TS

| | | |
|---------------------|---------------------|--------------------|
| 1.0000000000000000 | | |
| -7.9236880000000003 | -0.0000170000000000 | 9.8763220000000000 |
| 3.9615610000000001 | -6.8622589999999999 | 9.8761060000000001 |
| 3.9615469999999999 | 6.8621980000000002 | 9.8760700000000003 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1196047128441649 | 0.7419441368334390 | 0.2794578531477043 |
| 0.6220727731094087 | 0.2408229961106656 | 0.7793821456167649 |
| 0.8532806425955002 | 0.4667701366179173 | 0.3123165841621400 |
| 0.3471955990959188 | 0.9722426894837852 | 0.8266315921909282 |
| 0.8906814660446045 | 0.1967643267919073 | 0.0471165560389437 |
| 0.4021601555372385 | 0.6907646859492260 | 0.5536351694694659 |
| 0.7444880205741953 | 0.3631197857487152 | 0.2121689659755432 |
| 0.2495134089272142 | 0.8627651911663392 | 0.7110964344472634 |
| 0.0149627832736812 | 0.6364024549774996 | 0.1737856313148569 |
| 0.5126240008935454 | 0.1386846302838833 | 0.6694856827047460 |
| 0.2883500106079495 | 0.5945190931843669 | 0.4477325997783552 |
| 0.7897350916518420 | 0.0842445264958371 | 0.9416419962128941 |
| 0.2844056832638131 | 0.3656163340010039 | 0.6763621921139560 |
| 0.7822579273496615 | 0.8667787447567861 | 0.1768370476129206 |
| 0.7358123003540769 | 0.1416918642933425 | 0.4416922977251048 |
| 0.2413956792585381 | 0.6389619341903909 | 0.9411116829851522 |
| 0.3935935681423857 | 0.4649078546187724 | 0.7855789532214459 |
| 0.8904093830519315 | 0.9726577726267465 | 0.2790681787086058 |
| 0.1199475099622447 | 0.1987296104538316 | 0.8219399684320692 |
| 0.6195643499592904 | 0.7002171731363447 | 0.3153282727745008 |
| 0.3461325693595683 | 0.7448871014529743 | 0.0495103445084339 |
| 0.8446878344122837 | 0.2494070946236207 | 0.5480346462623089 |
| 0.5128332680193282 | 0.5963138987565912 | 0.2172303005491045 |
| 0.0187647047648127 | 0.0887153062455823 | 0.7083721891926729 |
| 0.2262814428889470 | 0.7832090244908585 | 0.1586660218133673 |
| 0.7296649758252016 | 0.2853041577557320 | 0.6626974021910144 |
| 0.2319779989994117 | 0.0834259265174921 | 0.8656672917566013 |
| 0.7350862258343653 | 0.5821863049066280 | 0.3295738054462163 |
| 0.9299024599679555 | 0.0815462290493869 | 0.1603752763064037 |
| 0.4335290651270469 | 0.5726283855492795 | 0.6658481237789573 |
| 0.6966695536048064 | 0.2561902904326345 | 0.3286867424146394 |
| 0.2088828971429066 | 0.7495765874079652 | 0.8247526169183246 |

0.4013929933164064 0.2568745794203409 0.6320530957630908
0.9004596046118181 0.7534139992996387 0.1462868291313697
0.4085650527579858 0.5518377562044989 0.3402123486397599
0.9045244691390977 0.0429870937318597 0.8356674882492143
0.1717627951742600 0.6708319517802153 0.3959816310367970
0.6663501344106635 0.1600266512795940 0.8992902303731327
0.4667262600332336 0.0190931775759751 0.7472442000114938
0.9743305363953141 0.5125467424743633 0.2414518450539234
0.8093094696040524 0.3174762554399067 0.0923727996105086
0.3433696341361170 0.8129323309600167 0.5945448466143333
0.4616790848637962 0.6605863717769864 0.1009522565173313
0.9687852444498972 0.1731681477482070 0.5804753714038782
0.1653501469911234 0.3205504692634094 0.7524389208072719
0.6606892110172282 0.8227996888630500 0.2534836931300575
0.8184300645525440 0.0210057169268296 0.3976918229857418
0.3166138304973387 0.5132656247930498 0.9044511609698986
0.0107073895324774 0.8624901009344441 0.3036812066112873
0.5139131857460981 0.3589021018865139 0.8132575256742314
0.8626285524738506 0.3760678762185847 0.4440600668033738
0.3754261087431559 0.8673075037074724 0.9489241432535778
0.0133354578896601 0.2226983330974477 0.9451929255187110
0.5276082009762462 0.7035629747096905 0.4485470243716350
0.6271930930566185 0.4795788205816365 0.1932389296589321
0.1374073159566294 0.9654042416978967 0.6689829142611075
0.1171883873760677 0.6208446091139450 0.0472093128173441
0.6129339628710326 0.1141306900677179 0.5443504365597889
0.2604872451343425 0.4741165022488616 0.5544953584843100
0.7572718944441803 0.9670190547297040 0.0538550192426825
0.0712817303664011 0.6514331283466532 0.2603499576265378
0.5690564909490590 0.1626855572455526 0.7486608164674209
0.8426684653038379 0.3990244715590805 0.2335141398561404
0.3249684416959582 0.9146474709425760 0.7471129142369080
0.8083969848611261 0.1694684565766451 0.9973425098726949
0.3112724419661319 0.6785033825477811 0.5004251627840475
0.0770212924809428 0.1755863460576492 0.7340898914485976
0.5528059298263983 0.6952674355714734 0.2322538811837873
0.3100453335478264 0.4129251820458393 0.7622636914635308
0.8011771613238494 0.9237533990775688 0.2596369776069025
0.3241990306582565 0.6652678953328461 0.9917642231521810
0.8113751904602324 0.1735924660206223 0.49437252711109045
0.3912907831700210 0.2642740478420436 0.1078202862543165
0.5054957244036444 0.1998977874431347 0.2837060735859609
0.4126836163100052 0.3504827699521229 0.2332739380149462
0.4301633554592499 0.2946953539417621 0.3806941745035743
0.3081799699784327 0.0638807267453601 0.3292763848679741
0.4140433908903063 0.0339311730903518 0.4192384764227057
0.2467192949367742 0.0674561635379476 0.4962766483288235
0.4839129148189230 0.1195476055380666 0.1719936688822870
0.1353736268301375 0.3080509363358743 0.2361979518304622
0.0994644121618933 0.1874665207755939 0.3688140887241715
0.1579497288763676 0.1647819086553639 0.2221545160554612
0.2137810249747929 0.3432697091351002 0.4794384034239485
0.1173092618004290 0.2816044057657621 0.4675848971027605
0.1718175983955419 0.4002904666207456 0.3443417485358964
0.3759201592157382 0.1293023013197470 0.1100368604597435
0.4216950157254757 0.2694598834556530 0.3118440839936767
0.3233217466920877 0.0989752150003582 0.4255091190118847
0.3095509199241846 0.2266662321777630 0.3661703511473604

| | | |
|--------------------|--------------------|--------------------|
| 0.2930077226749219 | 0.1676825454039630 | 0.2816648942890083 |
| 0.3930487616354057 | 0.1698700763693282 | 0.1610029621427103 |
| 0.1627564845390594 | 0.2094065764468596 | 0.2777013403130297 |
| 0.1953875624000005 | 0.3175398462533963 | 0.4171930241612714 |

Type B isomerisation, configuration P2 of the product

1

| | | |
|-----------|-----------|----------|
| -7.923688 | -0.000017 | 9.876322 |
| 3.961561 | -6.862259 | 9.876106 |
| 3.961547 | 6.862198 | 9.876070 |

Si Al O H C
23 1 48 15 7

Direct configuration= 1460

| | | |
|------------|------------|------------|
| 0.11825287 | 0.74113950 | 0.28236503 |
| 0.62074814 | 0.23761493 | 0.78264581 |
| 0.85020305 | 0.46667439 | 0.31418651 |
| 0.34382495 | 0.97153364 | 0.83011410 |
| 0.88759893 | 0.19541205 | 0.04989444 |
| 0.40186840 | 0.69083939 | 0.55552875 |
| 0.74315213 | 0.36283486 | 0.21432053 |
| 0.24613810 | 0.86162287 | 0.71401449 |
| 0.01513932 | 0.63301089 | 0.17764137 |
| 0.50982981 | 0.13801668 | 0.67207521 |
| 0.28687728 | 0.59382681 | 0.45080386 |
| 0.78801194 | 0.08373312 | 0.94266467 |
| 0.28177089 | 0.36589817 | 0.68001319 |
| 0.78253925 | 0.86452711 | 0.17681549 |
| 0.73424478 | 0.14013103 | 0.44483494 |
| 0.24045639 | 0.63721070 | 0.94382999 |
| 0.39342502 | 0.46441957 | 0.78690796 |
| 0.88823943 | 0.97163465 | 0.28072915 |
| 0.11842655 | 0.19788104 | 0.82423822 |
| 0.61714368 | 0.70116702 | 0.31658638 |
| 0.34431351 | 0.74457759 | 0.05230774 |
| 0.84407443 | 0.24697838 | 0.55027935 |
| 0.51016099 | 0.59516950 | 0.22065861 |
| 0.01957303 | 0.09001898 | 0.70643712 |
| 0.22440114 | 0.78312239 | 0.16135049 |
| 0.73046921 | 0.27944961 | 0.66750262 |
| 0.22934210 | 0.08277796 | 0.87068330 |
| 0.73406798 | 0.58386413 | 0.32787619 |
| 0.92860547 | 0.08091180 | 0.16283588 |
| 0.43352777 | 0.57169709 | 0.66752276 |
| 0.69621662 | 0.25665974 | 0.33252529 |
| 0.20727747 | 0.74616196 | 0.82738989 |
| 0.39935807 | 0.25761924 | 0.63556005 |
| 0.90027753 | 0.74916205 | 0.15005304 |
| 0.40628745 | 0.54938849 | 0.34329386 |
| 0.90064152 | 0.05067760 | 0.83206480 |
| 0.17036582 | 0.67100072 | 0.39883259 |
| 0.66128389 | 0.15792188 | 0.90524586 |
| 0.46288715 | 0.01901073 | 0.74849600 |
| 0.97411117 | 0.50874057 | 0.24714992 |
| 0.80623593 | 0.31615644 | 0.09525448 |
| 0.34223575 | 0.81138268 | 0.59854967 |
| 0.45949910 | 0.65880656 | 0.10403307 |
| 0.97112503 | 0.17619562 | 0.57748260 |
| 0.16340675 | 0.31996652 | 0.75777184 |

| | | |
|------------|------------|------------|
| 0.65935888 | 0.82321911 | 0.25212210 |
| 0.81459287 | 0.02001192 | 0.39932808 |
| 0.31826055 | 0.51069012 | 0.90781497 |
| 0.00802592 | 0.86104946 | 0.30621965 |
| 0.51316898 | 0.35704786 | 0.81456660 |
| 0.85452487 | 0.37595059 | 0.44684287 |
| 0.37433779 | 0.86675492 | 0.95188472 |
| 0.00910432 | 0.22186889 | 0.94621697 |
| 0.52795754 | 0.70332710 | 0.45099405 |
| 0.62569161 | 0.47924488 | 0.19623751 |
| 0.13238905 | 0.96150320 | 0.67406695 |
| 0.11767146 | 0.61529658 | 0.05147962 |
| 0.61009511 | 0.11442438 | 0.54644626 |
| 0.25727342 | 0.47483312 | 0.55883777 |
| 0.76221313 | 0.96179322 | 0.05097438 |
| 0.07178515 | 0.64895782 | 0.26323476 |
| 0.56719357 | 0.15978449 | 0.75219039 |
| 0.84276509 | 0.39956684 | 0.23269845 |
| 0.31912539 | 0.91315654 | 0.75349376 |
| 0.80371576 | 0.16708224 | 0.00288968 |
| 0.31211548 | 0.67756221 | 0.50171776 |
| 0.07945370 | 0.17455856 | 0.73363601 |
| 0.54835042 | 0.69506510 | 0.23613037 |
| 0.30762153 | 0.41323903 | 0.76602854 |
| 0.80036984 | 0.92324019 | 0.25874477 |
| 0.32183522 | 0.66512068 | 0.99470661 |
| 0.81145927 | 0.16835205 | 0.49894640 |
| 0.34371222 | 0.31408996 | 0.05954382 |
| 0.52625638 | 0.23208613 | 0.17581369 |
| 0.42512101 | 0.37879891 | 0.18323480 |
| 0.49555267 | 0.28230704 | 0.30017844 |
| 0.46116233 | 0.04089025 | 0.31117796 |
| 0.44547727 | 0.08898488 | 0.43266508 |
| 0.32319707 | 0.05018958 | 0.43548549 |
| 0.45036794 | 0.17455507 | 0.09789726 |
| 0.11000898 | 0.32312776 | 0.27332907 |
| 0.12913352 | 0.18711487 | 0.38865897 |
| 0.13402644 | 0.18853013 | 0.24130997 |
| 0.31457318 | 0.29224587 | 0.46135612 |
| 0.19013206 | 0.25111503 | 0.47547686 |
| 0.21618407 | 0.39057567 | 0.36954452 |
| 0.31094199 | 0.18059391 | 0.08198474 |
| 0.45506238 | 0.28412062 | 0.23739407 |
| 0.39680598 | 0.09157690 | 0.37641980 |
| 0.34702999 | 0.23224359 | 0.31196956 |
| 0.28713809 | 0.22305467 | 0.23971676 |
| 0.35193371 | 0.21739343 | 0.11515506 |
| 0.16049208 | 0.22428556 | 0.28916398 |
| 0.26063007 | 0.29496024 | 0.41057545 |

Type B isomerisation, configuration R3 of the reactant

| | | | | |
|-----------|-----------|----------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |

Direct configuration= 1005

| | | |
|------------|------------|------------|
| 0.11715216 | 0.74412564 | 0.28990263 |
| 0.61813495 | 0.23890985 | 0.79088941 |
| 0.85076645 | 0.46718879 | 0.32255211 |
| 0.34187178 | 0.97370447 | 0.83785473 |
| 0.88652825 | 0.19841912 | 0.05759845 |
| 0.40059029 | 0.69197427 | 0.56394529 |
| 0.74254867 | 0.36467239 | 0.22268558 |
| 0.24350913 | 0.86294550 | 0.72226643 |
| 0.01355796 | 0.63547970 | 0.18487106 |
| 0.50870556 | 0.13905791 | 0.68102561 |
| 0.28604254 | 0.59604272 | 0.45815013 |
| 0.78681295 | 0.08576914 | 0.95153831 |
| 0.28045790 | 0.36773270 | 0.68780138 |
| 0.78167261 | 0.86633410 | 0.18523231 |
| 0.73337053 | 0.14328267 | 0.45170062 |
| 0.23908904 | 0.63886472 | 0.95202355 |
| 0.39055116 | 0.46584514 | 0.79572136 |
| 0.88750001 | 0.97410010 | 0.28875645 |
| 0.11754965 | 0.19917844 | 0.83261346 |
| 0.61689695 | 0.70164942 | 0.32530178 |
| 0.34330465 | 0.74693473 | 0.05996108 |
| 0.84215261 | 0.24985764 | 0.55774074 |
| 0.50974180 | 0.59782844 | 0.22786280 |
| 0.01779970 | 0.08968794 | 0.71578313 |
| 0.22461138 | 0.78644153 | 0.16983777 |
| 0.72441695 | 0.28171188 | 0.67304648 |
| 0.22950504 | 0.08572270 | 0.88032800 |
| 0.73218763 | 0.58374455 | 0.33446868 |
| 0.92717875 | 0.08328547 | 0.17034530 |
| 0.43185974 | 0.57166712 | 0.67474554 |
| 0.69346252 | 0.25869045 | 0.33945716 |
| 0.20616121 | 0.74699873 | 0.83507325 |
| 0.39917258 | 0.25956781 | 0.64535282 |
| 0.89886637 | 0.75216254 | 0.15567839 |
| 0.40568273 | 0.55277960 | 0.35020504 |
| 0.90017967 | 0.04886132 | 0.84340072 |
| 0.16943912 | 0.67318943 | 0.40630972 |
| 0.66075460 | 0.16037915 | 0.91255936 |
| 0.46149293 | 0.01990229 | 0.75525060 |
| 0.97189179 | 0.51249635 | 0.25512122 |
| 0.80527492 | 0.31918256 | 0.10275339 |
| 0.34167157 | 0.81255861 | 0.60701972 |
| 0.45934758 | 0.66265762 | 0.11092042 |
| 0.96565121 | 0.17801619 | 0.59047793 |
| 0.16203814 | 0.32152362 | 0.76361725 |
| 0.65851202 | 0.82422265 | 0.26148776 |
| 0.81281175 | 0.02240447 | 0.40711859 |
| 0.31766712 | 0.51324935 | 0.91539065 |
| 0.00870750 | 0.86524968 | 0.31375853 |
| 0.50957583 | 0.35724760 | 0.82366251 |
| 0.85246008 | 0.37991859 | 0.45682584 |
| 0.37321017 | 0.86983549 | 0.96016027 |
| 0.00872340 | 0.22425761 | 0.95453572 |
| 0.52673028 | 0.70481045 | 0.45914129 |
| 0.62668178 | 0.48345317 | 0.20371908 |
| 0.12915469 | 0.96078612 | 0.68242556 |
| 0.11595831 | 0.61830727 | 0.05878003 |
| 0.61117557 | 0.11678493 | 0.55658519 |

| | | |
|------------|------------|------------|
| 0.25758152 | 0.47696868 | 0.56627851 |
| 0.75653231 | 0.96629391 | 0.06200400 |
| 0.06943933 | 0.65455734 | 0.26917086 |
| 0.56292571 | 0.15696621 | 0.76720381 |
| 0.84298827 | 0.39845580 | 0.24273644 |
| 0.31424287 | 0.91579417 | 0.76333086 |
| 0.80300241 | 0.17031784 | 0.00989136 |
| 0.31086532 | 0.68132506 | 0.50792375 |
| 0.07962822 | 0.17125158 | 0.74472188 |
| 0.54567214 | 0.70009090 | 0.24354180 |
| 0.30344853 | 0.41523325 | 0.77587951 |
| 0.80096275 | 0.92334647 | 0.26755238 |
| 0.31978283 | 0.66862964 | 0.00246476 |
| 0.81280365 | 0.17253966 | 0.50209433 |
| 0.23913825 | 0.19222160 | 0.46934843 |
| 0.31588131 | 0.94782408 | 0.33935081 |
| 0.25417329 | 0.96576823 | 0.22262472 |
| 0.40881825 | 0.88669225 | 0.21814998 |
| 0.42823417 | 0.21051396 | 0.30813512 |
| 0.49622140 | 0.02431294 | 0.26492672 |
| 0.50680557 | 0.15336342 | 0.12872121 |
| 0.20223553 | 0.12455522 | 0.39750243 |
| 0.34714316 | 0.35548758 | 0.13114929 |
| 0.24733960 | 0.37900248 | 0.27317616 |
| 0.21424624 | 0.30572224 | 0.20316558 |
| 0.34717470 | 0.23561873 | 0.02542066 |
| 0.27857905 | 0.12683719 | 0.03743808 |
| 0.43857937 | 0.10478667 | 0.98194690 |
| 0.32988350 | 0.04514114 | 0.45551739 |
| 0.33103934 | 0.96556435 | 0.24221067 |
| 0.44626467 | 0.10423739 | 0.20659459 |
| 0.37571673 | 0.07052931 | 0.16678677 |
| 0.35930458 | 0.19464361 | 0.28924148 |
| 0.27893177 | 0.13474574 | 0.40866407 |
| 0.28880476 | 0.31490991 | 0.21910900 |
| 0.35316049 | 0.13960200 | 0.04938363 |

Type B isomerisation, configuration TS3 of the TS

| | | |
|---------------------|---------------------|--------------------|
| 1.0000000000000000 | | |
| -7.9236880000000003 | -0.0000170000000000 | 9.8763220000000000 |
| 3.9615610000000001 | -6.8622589999999999 | 9.8761060000000001 |
| 3.9615469999999999 | 6.8621980000000002 | 9.8760700000000003 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1139016838835465 | 0.7451750087832040 | 0.2908764306357142 |
| 0.6211303820923700 | 0.2399559618394513 | 0.7858683544492733 |
| 0.8501884368640654 | 0.4692242201823266 | 0.3261650162489381 |
| 0.3406893736048475 | 0.9760841210729836 | 0.8379989922587393 |
| 0.8846692843320587 | 0.1985693348588076 | 0.0587447857756537 |
| 0.3979075003805318 | 0.6938687777077848 | 0.5649108539877917 |
| 0.7376366356336665 | 0.3677327923507804 | 0.2206531068979371 |
| 0.2444711587590646 | 0.8617471731418936 | 0.7254550669735335 |
| 0.0139717685693142 | 0.6361252516067022 | 0.1837787778567325 |
| 0.5079074030282233 | 0.1407560407308018 | 0.6801175142686591 |
| 0.2848852592720942 | 0.5966981588781498 | 0.4596125696154315 |
| 0.7855534913317151 | 0.0888043998643779 | 0.9550986133097346 |
| 0.2778951821601569 | 0.3708264167945016 | 0.6893999870531481 |

| | | |
|--------------------|--------------------|--------------------|
| 0.7844669020616226 | 0.8650900214958117 | 0.1808229262660253 |
| 0.7290665178797207 | 0.1435160208143077 | 0.4497540784370025 |
| 0.2457363611504068 | 0.6369582406480290 | 0.9537399011056221 |
| 0.3919348142354289 | 0.4674943332063601 | 0.7944135265128364 |
| 0.8883113893947773 | 0.9746391564385870 | 0.2873066026408221 |
| 0.1165966632903288 | 0.2020011855316484 | 0.8267813160945141 |
| 0.6223870101380028 | 0.6981191819151745 | 0.3300733906378492 |
| 0.3418380231233170 | 0.7506610099266759 | 0.0608385714772774 |
| 0.8438013293961945 | 0.2448411104659756 | 0.5561062748113392 |
| 0.5115056065841925 | 0.5957866587842792 | 0.2288317500965058 |
| 0.0197651218740267 | 0.0902045667687283 | 0.7175170092575112 |
| 0.2173901455081725 | 0.7868601587344457 | 0.1666829915840840 |
| 0.7262184758760678 | 0.2859872262376822 | 0.6676339099404107 |
| 0.2261946752173734 | 0.0879510072208374 | 0.8767215116022650 |
| 0.7369836547637663 | 0.5841233624785549 | 0.3594499524908812 |
| 0.9293400093681696 | 0.0843696771215455 | 0.1702215942288769 |
| 0.4340806705525940 | 0.5741381368389191 | 0.6745508052562351 |
| 0.6929593611336031 | 0.2586284750401537 | 0.3359275930881721 |
| 0.2098970308452383 | 0.7445434812380702 | 0.8379210065582350 |
| 0.3969602920672354 | 0.2618112376082309 | 0.6494769960805246 |
| 0.9016564811611633 | 0.7525023927214500 | 0.1467326791803350 |
| 0.4077050408500756 | 0.5549893933796095 | 0.3536941123508560 |
| 0.9073598465283309 | 0.0549517609860209 | 0.8531565637460663 |
| 0.1708662062118511 | 0.6731447691405364 | 0.4039854061986177 |
| 0.6652601604096273 | 0.1632345126362783 | 0.9068896751755318 |
| 0.4605032327484892 | 0.0220294272157242 | 0.7563916303677296 |
| 0.9720962636423195 | 0.5131510969587657 | 0.2498874890158364 |
| 0.8133764593939676 | 0.3212279034063418 | 0.1015181951678383 |
| 0.3398241558142167 | 0.8143127724326018 | 0.6079302691366809 |
| 0.4549283143893001 | 0.6738166893137376 | 0.1166836826335508 |
| 0.9633691608981214 | 0.1647276071737710 | 0.5943904971073908 |
| 0.1592077712029643 | 0.3251687129521695 | 0.7676039652683839 |
| 0.6624847758334282 | 0.8219102827577394 | 0.2618093843043779 |
| 0.8071440372668056 | 0.0223473095510576 | 0.4055538399301662 |
| 0.3231340861300646 | 0.5113785364448975 | 0.9165722393068587 |
| 0.0078657984612058 | 0.8667278625183843 | 0.3174664425487693 |
| 0.5104609329888745 | 0.3565674190486396 | 0.8195662915675423 |
| 0.8685859847186693 | 0.3682726402368632 | 0.4506740264273797 |
| 0.3696020620093605 | 0.8743739325800819 | 0.9618014670848736 |
| 0.0020913540824679 | 0.2212384226714938 | 0.9466252882806619 |
| 0.5200401685869291 | 0.7118370493349339 | 0.4559941687808178 |
| 0.6162348949056846 | 0.4763352465688159 | 0.1966904028849706 |
| 0.1279305366627274 | 0.9582927289552214 | 0.6894859729902245 |
| 0.1241459614366322 | 0.6157919177287720 | 0.0629730646016135 |
| 0.6047389584507952 | 0.1198109462078823 | 0.5523719147396430 |
| 0.2554556046963739 | 0.4767202373345813 | 0.5656713279368746 |
| 0.7523147370589237 | 0.9674264507532109 | 0.0607793578468004 |
| 0.0599686436822953 | 0.6572969198440486 | 0.2747872547947715 |
| 0.5705939204544487 | 0.1561580606468518 | 0.7600947730533990 |
| 0.8239125794405362 | 0.4162791861827556 | 0.2449555621379751 |
| 0.3173465483505913 | 0.9148844426191249 | 0.7631956373556676 |
| 0.7894296570267206 | 0.1714466614002800 | 0.0246270446887325 |
| 0.3055343288445541 | 0.6806943138416133 | 0.5142525999344094 |
| 0.0867514600758477 | 0.1794750775405886 | 0.7290120401606003 |
| 0.5688877183214854 | 0.6812677750717667 | 0.2431678631342837 |
| 0.3006048087386251 | 0.4229282678804668 | 0.7738930839328440 |
| 0.8069602161389170 | 0.9222700327115749 | 0.2606320229142162 |
| 0.3292768190621395 | 0.6667507976073120 | 0.0007650840834576 |

| | | |
|--------------------|--------------------|--------------------|
| 0.8078822317089897 | 0.1715344454274380 | 0.5018432846084946 |
| 0.2374340132218786 | 0.1788310993055923 | 0.4547061002710847 |
| 0.3884237181277224 | 0.9129445412558632 | 0.3353828386065401 |
| 0.2634662890455066 | 0.9666990590568052 | 0.2764186117164539 |
| 0.4121662713573629 | 0.9000357028873189 | 0.1919564595589619 |
| 0.4076025072274129 | 0.1906831024196886 | 0.2755768335087734 |
| 0.5293466544448546 | 0.0345955799083022 | 0.2611413556846124 |
| 0.5256918436380332 | 0.1676489285818540 | 0.1205838240888099 |
| 0.1888100484597490 | 0.0927526914429798 | 0.4126562340739217 |
| 0.3110862149761168 | 0.3443168459686485 | 0.1233173705603284 |
| 0.2210688746528918 | 0.3547195747139249 | 0.2728309949755658 |
| 0.1789865917127901 | 0.2943724550940951 | 0.1966317507874823 |
| 0.3786182066084233 | 0.2231268417495637 | 0.0124119556762304 |
| 0.2592976693057287 | 0.1536120811343250 | 0.0768847886688279 |
| 0.4096809661801755 | 0.0734588523336904 | 0.0104539974771993 |
| 0.3301801743082243 | 0.0302366148115988 | 0.4447482430549482 |
| 0.3600288247723547 | 0.9578569990002771 | 0.2526382920996962 |
| 0.4817785419142958 | 0.1010910701944326 | 0.1944635627055377 |
| 0.3827639488756769 | 0.0805622885074577 | 0.1850443815262342 |
| 0.3275550270942137 | 0.1722143171670557 | 0.2702885419165590 |
| 0.2685141767808799 | 0.1140572386772238 | 0.4035434893012365 |
| 0.2564139758261936 | 0.2994535658904794 | 0.2109808710362305 |
| 0.3553071211928583 | 0.1378390719924603 | 0.0642318872394125 |

Type B isomerisation, configuration P3 of the product

| | | | | |
|----------------------------|------------|------------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |
| Direct configuration= 2155 | | | | |
| 0.12388536 | 0.74204206 | 0.28813775 | | |
| 0.62683132 | 0.23883088 | 0.78797274 | | |
| 0.85727807 | 0.46629518 | 0.32122591 | | |
| 0.34995346 | 0.97233607 | 0.83559871 | | |
| 0.89540312 | 0.19640382 | 0.05618215 | | |
| 0.40426659 | 0.69311565 | 0.56138993 | | |
| 0.74896955 | 0.36333261 | 0.22094809 | | |
| 0.25170918 | 0.86137329 | 0.72111284 | | |
| 0.01923514 | 0.63686910 | 0.18096874 | | |
| 0.51741199 | 0.13761490 | 0.67959799 | | |
| 0.29286042 | 0.59471240 | 0.45578635 | | |
| 0.79068146 | 0.08549396 | 0.95128077 | | |
| 0.28828077 | 0.36600142 | 0.68596067 | | |
| 0.78722359 | 0.86599964 | 0.18352579 | | |
| 0.74075099 | 0.14088342 | 0.45015410 | | |
| 0.24801864 | 0.63599866 | 0.95073714 | | |
| 0.39635560 | 0.46512532 | 0.79376167 | | |
| 0.89570258 | 0.97229476 | 0.28664901 | | |
| 0.12374826 | 0.19840076 | 0.83079180 | | |
| 0.62357081 | 0.69958296 | 0.32562828 | | |
| 0.35083799 | 0.74517086 | 0.05858021 | | |
| 0.85147134 | 0.24648795 | 0.55532914 | | |
| 0.51741936 | 0.59671752 | 0.22603727 | | |
| 0.02160561 | 0.08650500 | 0.71919857 | | |
| 0.23109568 | 0.78379083 | 0.16797617 | | |
| 0.73735079 | 0.27880611 | 0.67160463 | | |

| | | |
|------------|------------|------------|
| 0.23548830 | 0.08369987 | 0.87628280 |
| 0.73826895 | 0.58013702 | 0.34029431 |
| 0.93647589 | 0.08159152 | 0.16895718 |
| 0.43208173 | 0.57487601 | 0.67480687 |
| 0.70159106 | 0.25720648 | 0.33854480 |
| 0.21663507 | 0.74415445 | 0.83311852 |
| 0.40774851 | 0.25826412 | 0.64401284 |
| 0.90534064 | 0.75289996 | 0.15041741 |
| 0.41272592 | 0.55192301 | 0.34806051 |
| 0.90174221 | 0.04685630 | 0.84164333 |
| 0.17561605 | 0.66908223 | 0.40468441 |
| 0.66615070 | 0.16447702 | 0.91139156 |
| 0.46926764 | 0.01912705 | 0.75459537 |
| 0.97816668 | 0.51280144 | 0.25092724 |
| 0.81340146 | 0.31685220 | 0.10167994 |
| 0.34487744 | 0.81527129 | 0.60221890 |
| 0.46700080 | 0.66191809 | 0.10914834 |
| 0.97723989 | 0.17196619 | 0.58662266 |
| 0.16971513 | 0.31963578 | 0.75914387 |
| 0.66700509 | 0.82060446 | 0.26288136 |
| 0.82109022 | 0.02056806 | 0.40510353 |
| 0.32486852 | 0.50916695 | 0.91591732 |
| 0.01596479 | 0.86293374 | 0.31300595 |
| 0.51928294 | 0.35987040 | 0.81418605 |
| 0.86833529 | 0.37373035 | 0.45204757 |
| 0.37920431 | 0.86816399 | 0.95816799 |
| 0.01728985 | 0.22411063 | 0.95371207 |
| 0.53189851 | 0.70292456 | 0.45887520 |
| 0.63269069 | 0.48069508 | 0.20162518 |
| 0.13503481 | 0.95933128 | 0.68537641 |
| 0.12362166 | 0.61679600 | 0.05665860 |
| 0.61874116 | 0.11441833 | 0.55458769 |
| 0.26607478 | 0.47510735 | 0.56417926 |
| 0.75997134 | 0.96653135 | 0.06152718 |
| 0.07417343 | 0.65407435 | 0.26706464 |
| 0.57538305 | 0.15642461 | 0.76134089 |
| 0.84874808 | 0.39889294 | 0.24072289 |
| 0.32473424 | 0.91421283 | 0.75906531 |
| 0.81413804 | 0.16703935 | 0.00726839 |
| 0.31504797 | 0.68198996 | 0.50519641 |
| 0.07999802 | 0.17240958 | 0.74567162 |
| 0.55649694 | 0.69559966 | 0.24226744 |
| 0.30879711 | 0.41383194 | 0.77539068 |
| 0.80997159 | 0.92198135 | 0.26430091 |
| 0.32837392 | 0.66502711 | 0.00192587 |
| 0.82140986 | 0.16934144 | 0.50054258 |
| 0.26396286 | 0.17586380 | 0.46077451 |
| 0.22014931 | 0.95479993 | 0.36512691 |
| 0.07909609 | 0.06472487 | 0.34999897 |
| 0.17309105 | 0.98735899 | 0.23800764 |
| 0.42449243 | 0.13387548 | 0.10768856 |
| 0.41960000 | 0.00323158 | 0.23866062 |
| 0.37797194 | 0.01504595 | 0.11445884 |
| 0.12577832 | 0.16263514 | 0.46736686 |
| 0.31094371 | 0.32809939 | 0.14090228 |
| 0.29070835 | 0.33868675 | 0.28776626 |
| 0.16482499 | 0.37513253 | 0.23551962 |
| 0.23085832 | 0.28038603 | 0.05522934 |

| | | |
|------------|------------|------------|
| 0.08603857 | 0.26304722 | 0.15368355 |
| 0.18528247 | 0.15936093 | 0.06793951 |
| 0.25314586 | 0.03802275 | 0.45530840 |
| 0.17355057 | 0.02765979 | 0.29969174 |
| 0.37522794 | 0.06652458 | 0.16804747 |
| 0.23636532 | 0.12764400 | 0.22350852 |
| 0.24250024 | 0.19100638 | 0.29547118 |
| 0.22902360 | 0.13749569 | 0.42302974 |
| 0.25751917 | 0.31301001 | 0.23700151 |
| 0.18158847 | 0.21379966 | 0.11879268 |

Type B isomerisation, configuration R4 of the reactant

| | | | | |
|-----------|-----------|----------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |

Direct configuration= 1458

| | | |
|------------|------------|------------|
| 0.12302348 | 0.74470762 | 0.28554197 |
| 0.62242485 | 0.23835808 | 0.78707196 |
| 0.85499407 | 0.46748827 | 0.31994180 |
| 0.35017326 | 0.97164805 | 0.83201352 |
| 0.89662290 | 0.19715238 | 0.05377746 |
| 0.40412482 | 0.69014606 | 0.55888331 |
| 0.74831124 | 0.36433325 | 0.21863226 |
| 0.24768370 | 0.86187911 | 0.71973971 |
| 0.01673839 | 0.63800723 | 0.17895068 |
| 0.51561270 | 0.13742329 | 0.67930362 |
| 0.29260571 | 0.59554275 | 0.45292830 |
| 0.79483940 | 0.08379928 | 0.94777506 |
| 0.28714209 | 0.36537455 | 0.68418177 |
| 0.78800141 | 0.86521949 | 0.18064304 |
| 0.74141603 | 0.14216896 | 0.44696238 |
| 0.24382103 | 0.63950948 | 0.94821672 |
| 0.39487756 | 0.46316968 | 0.79131810 |
| 0.89657709 | 0.97188670 | 0.28540531 |
| 0.12338074 | 0.19809336 | 0.83013892 |
| 0.62150030 | 0.70149125 | 0.32226198 |
| 0.35019261 | 0.74571812 | 0.05542975 |
| 0.84709637 | 0.24822742 | 0.55341543 |
| 0.51673551 | 0.59806743 | 0.22314357 |
| 0.02100360 | 0.08469545 | 0.71720837 |
| 0.23093496 | 0.78490204 | 0.16503704 |
| 0.72343737 | 0.28198287 | 0.66217985 |
| 0.23828128 | 0.08528667 | 0.87382944 |
| 0.73452996 | 0.58031272 | 0.33634258 |
| 0.93495575 | 0.08290111 | 0.16815278 |
| 0.43462746 | 0.56484637 | 0.66544449 |
| 0.70043569 | 0.25820689 | 0.33573381 |
| 0.20370970 | 0.75156366 | 0.83650163 |
| 0.40610646 | 0.25747692 | 0.64217215 |
| 0.90381160 | 0.75259009 | 0.14236824 |
| 0.41329717 | 0.55241409 | 0.34606708 |
| 0.90790156 | 0.03570460 | 0.84446820 |
| 0.17561650 | 0.66712997 | 0.40128770 |
| 0.67348562 | 0.16469315 | 0.90306269 |
| 0.46956534 | 0.01725941 | 0.74807876 |

| | | |
|------------|------------|------------|
| 0.97518062 | 0.51460728 | 0.25142638 |
| 0.81381303 | 0.31783440 | 0.09895536 |
| 0.34695626 | 0.80495878 | 0.61017871 |
| 0.46588596 | 0.66136126 | 0.10646895 |
| 0.96626392 | 0.17631920 | 0.59414656 |
| 0.16755514 | 0.32011293 | 0.75457517 |
| 0.66746880 | 0.82075618 | 0.26126871 |
| 0.81676477 | 0.02063878 | 0.40305900 |
| 0.32183471 | 0.51683016 | 0.90673373 |
| 0.02004116 | 0.86810546 | 0.31231871 |
| 0.51477972 | 0.35719258 | 0.81970605 |
| 0.86436693 | 0.37606952 | 0.45121691 |
| 0.37942440 | 0.86887599 | 0.95520669 |
| 0.02179141 | 0.22378495 | 0.95600423 |
| 0.53004627 | 0.70475761 | 0.45557593 |
| 0.63331667 | 0.48284820 | 0.19858496 |
| 0.13714491 | 0.96234269 | 0.67369941 |
| 0.12403187 | 0.61290954 | 0.05781978 |
| 0.62124321 | 0.11777868 | 0.55568396 |
| 0.26682511 | 0.47702960 | 0.56381344 |
| 0.75679890 | 0.97088728 | 0.06275379 |
| 0.06674710 | 0.66299682 | 0.26385932 |
| 0.56490086 | 0.15402853 | 0.76998997 |
| 0.84939972 | 0.39842345 | 0.23846107 |
| 0.31908507 | 0.91556482 | 0.75888701 |
| 0.82016438 | 0.16836638 | 0.99923355 |
| 0.31270134 | 0.68611546 | 0.50016586 |
| 0.07748190 | 0.16690243 | 0.75132249 |
| 0.55388507 | 0.69923803 | 0.23811748 |
| 0.30613705 | 0.40782902 | 0.77914641 |
| 0.81778589 | 0.91470377 | 0.26201877 |
| 0.32650611 | 0.66818362 | 0.99704761 |
| 0.82831565 | 0.16947421 | 0.49058602 |
| 0.11446228 | 0.28847777 | 0.37741820 |
| 0.05358548 | 0.32692978 | 0.10462460 |
| 0.14153699 | 0.35011097 | 0.16232712 |
| 0.20472043 | 0.33532789 | 0.00978294 |
| 0.14907266 | 0.06286833 | 0.45710500 |
| 0.03781191 | 0.17354929 | 0.31565483 |
| 0.13231261 | 0.02470829 | 0.29760974 |
| 0.23668176 | 0.20851294 | 0.44074977 |
| 0.36847222 | 0.99181600 | 0.41811044 |
| 0.39568240 | 0.05079456 | 0.25843960 |
| 0.33069833 | 0.92777467 | 0.34264133 |
| 0.25452333 | 0.09374272 | 0.02171242 |
| 0.32694089 | 0.00312484 | 0.13880885 |
| 0.36356666 | 0.14107797 | 0.02639752 |
| 0.26814609 | 0.26446414 | 0.28043283 |
| 0.14912347 | 0.30224617 | 0.10228140 |
| 0.13033507 | 0.11744647 | 0.28265409 |
| 0.19006282 | 0.17149559 | 0.15750654 |
| 0.20566589 | 0.10252796 | 0.36718966 |
| 0.20581123 | 0.22364729 | 0.36472747 |
| 0.33217760 | 0.01362300 | 0.34385781 |
| 0.29193448 | 0.09668937 | 0.08664544 |

Type B isomerisation, configuration TS4 of the TS
1.00000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236880000000003 | -0.0000170000000000 | 9.8763220000000000 |
| 3.9615610000000001 | -6.8622589999999999 | 9.8761060000000001 |
| 3.9615469999999999 | 6.8621980000000002 | 9.8760700000000003 |

| | | | | | |
|----|----|----|----|---|--|
| Si | Al | O | H | C | |
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1204880098958795 | 0.7481613148495663 | 0.2817860542732933 |
| 0.6236393819054625 | 0.2444970052899319 | 0.7803220312985752 |
| 0.8581010225314842 | 0.4697419482646112 | 0.3134232886370742 |
| 0.3465490686935336 | 0.9804434812213989 | 0.8292741844763437 |
| 0.8930868999867643 | 0.2037853373688521 | 0.0467717725079203 |
| 0.4057304311796120 | 0.6938481469089867 | 0.5566111050382335 |
| 0.7459238285077584 | 0.3699869485622342 | 0.2125227314726811 |
| 0.2502807820645640 | 0.8664161174973066 | 0.7153260909424349 |
| 0.0172527880316636 | 0.6411638063294643 | 0.1778492208597594 |
| 0.5141304100839658 | 0.1440037909317917 | 0.6704275976305872 |
| 0.2922049510640856 | 0.6029828409163522 | 0.4483090177240656 |
| 0.7932946727935970 | 0.0860353737984580 | 0.9438508616336073 |
| 0.2855061201046212 | 0.3711496444242403 | 0.6783852221424105 |
| 0.7878752248040325 | 0.8691514213038709 | 0.1771730854077958 |
| 0.7369651644964712 | 0.1476106882174372 | 0.4414107852237400 |
| 0.2477249125400910 | 0.6432172022983300 | 0.9438433713145806 |
| 0.3923592809999649 | 0.4656637169672886 | 0.7902164865694994 |
| 0.8969084525027379 | 0.9794877288048048 | 0.2775426643649859 |
| 0.1211524897018925 | 0.2051899356514805 | 0.8220122592253770 |
| 0.6249558257450296 | 0.7024889251205694 | 0.3216670236584452 |
| 0.3507631811857863 | 0.7502402394266451 | 0.0487288191188631 |
| 0.8454897142269729 | 0.2528360841089223 | 0.5495729632868839 |
| 0.5162035472007240 | 0.6041478883221026 | 0.2192565236928963 |
| 0.0213280362409440 | 0.0879819568808812 | 0.7122827311974232 |
| 0.2269154153026350 | 0.7814398327147128 | 0.1573094945844255 |
| 0.7278731037508430 | 0.2920173919478598 | 0.6604471002481097 |
| 0.2338595939403729 | 0.0933265152542144 | 0.8685137673625716 |
| 0.7392162049793614 | 0.5833047007324599 | 0.3346761009473410 |
| 0.9353851714951488 | 0.0900954939346785 | 0.1601070918242266 |
| 0.4297839239990113 | 0.5714813961511315 | 0.6666687263579787 |
| 0.6981111076106584 | 0.2635320060812983 | 0.3295620121574234 |
| 0.2085522998903893 | 0.7544844347269319 | 0.8303044576259773 |
| 0.4042067020264893 | 0.2640093072342005 | 0.6338879120845577 |
| 0.9041959212571435 | 0.7560978984325508 | 0.1415935617544766 |
| 0.4114285669401438 | 0.5591258509251610 | 0.3411642250727696 |
| 0.9093616202473843 | 0.0397734995611862 | 0.8410378882489998 |
| 0.1751703678321995 | 0.6794101551159166 | 0.3968066299811898 |
| 0.6729316710932530 | 0.1646160863318271 | 0.8970853665440660 |
| 0.4669696150168857 | 0.0248734388295491 | 0.7465106748253726 |
| 0.9783117794872596 | 0.5164979603002144 | 0.2424587450245912 |
| 0.8097125771931462 | 0.3236792191491751 | 0.0929796519961969 |
| 0.3484002504804112 | 0.8132342685857935 | 0.6019936817004817 |
| 0.4651917432439915 | 0.6725656327760037 | 0.1027786641164078 |
| 0.9664664173259566 | 0.1721558731354274 | 0.5873019241150665 |
| 0.1651846712610130 | 0.3274368672078008 | 0.7458253801757280 |
| 0.6680181305595603 | 0.8236950958238367 | 0.2609252867059851 |
| 0.8198522692566721 | 0.0274475624139240 | 0.3961371947789964 |
| 0.3183634243862952 | 0.5180437461506061 | 0.9063610131149250 |
| 0.0201528891777126 | 0.8745579704855561 | 0.3038908935785848 |
| 0.5145305263092457 | 0.3614400762501058 | 0.8153238368884232 |
| 0.8696200521718732 | 0.3766070471975009 | 0.4441290315999647 |
| 0.3744200229580990 | 0.8766596086261933 | 0.9523867411978483 |

| | | |
|--------------------|--------------------|--------------------|
| 0.0144993971596499 | 0.2328406709981383 | 0.9442933382360602 |
| 0.5344638686127796 | 0.7028918108968356 | 0.4562980814708627 |
| 0.6301710729602520 | 0.4880377312189517 | 0.1931176632659167 |
| 0.1391451240680675 | 0.9654564744832550 | 0.6670770906089917 |
| 0.1278126837062251 | 0.6252654675376137 | 0.0564165939931606 |
| 0.6153855709312386 | 0.1196459897451749 | 0.5455671267170248 |
| 0.2651650255597759 | 0.4854768686594412 | 0.5591609463099801 |
| 0.7564969673288365 | 0.9713070437754547 | 0.0574402425624281 |
| 0.0602649370816029 | 0.6626523734586612 | 0.2711814562485874 |
| 0.5716149359307082 | 0.1639228114222613 | 0.7517372791113123 |
| 0.8451267654020544 | 0.4049576742225344 | 0.2333420031340595 |
| 0.3190730360538415 | 0.9230893166521198 | 0.7534719696325334 |
| 0.8139799888570003 | 0.1712611688012147 | 0.9981376113705438 |
| 0.3146519696674316 | 0.6934657385293838 | 0.4944870740439472 |
| 0.0790017226271893 | 0.1735334994615698 | 0.7396638015827801 |
| 0.5559103515361232 | 0.7009684407255821 | 0.2384485828988209 |
| 0.3063431620820371 | 0.4111909598974564 | 0.7735122675421241 |
| 0.8156812469005771 | 0.9239269065055412 | 0.2555444539262975 |
| 0.3383964492302158 | 0.6699783608235760 | 0.9845720884516479 |
| 0.8163582055878762 | 0.1760529435186350 | 0.4931722438802162 |
| 0.1518756543936745 | 0.2056745823210828 | 0.4473277690155817 |
| 0.0416929604732864 | 0.2189657510602926 | 0.2039858946384883 |
| 0.0522674344784752 | 0.2485670569994400 | 0.3247263690451264 |
| 0.1640538771237539 | 0.2683097868166390 | 0.1805199939328298 |
| 0.2226633245687555 | 0.9932215314601018 | 0.4694892859773837 |
| 0.0561087506427609 | 0.0448120641967697 | 0.4717510996379269 |
| 0.1608038806012252 | 0.9064709080527598 | 0.4220306853110687 |
| 0.3035437883117600 | 0.1388623853928563 | 0.4556921121263116 |
| 0.4390783610749252 | 0.9562534077098948 | 0.3891581385471012 |
| 0.4332036409029109 | 1.0277806235490197 | 0.2359869234957380 |
| 0.3919378562725678 | 0.8916165855109265 | 0.3213346206951643 |
| 0.1777236937914110 | 0.0436683438939381 | 0.1347406019699030 |
| 0.2868013939094445 | 0.9289557846101363 | 0.2074026367116020 |
| 0.3131497734125027 | 0.0713251499396762 | 0.1119571958331164 |
| 0.2753740113871188 | 0.2331421118273888 | 0.3133403692070871 |
| 0.1045252772155551 | 0.2120947687973514 | 0.2473464717137913 |
| 0.1335043154577764 | 0.0048710621002256 | 0.4042526860051924 |
| 0.1773275565206953 | 0.0807141270936540 | 0.2845497239365644 |
| 0.2593673695730193 | 0.0530878131460719 | 0.3712402545429023 |
| 0.2454968493093756 | 0.1655670762126297 | 0.3986093649455931 |
| 0.3887571814669332 | 0.9770231950327020 | 0.3268858774511964 |
| 0.2437551835802475 | 0.0269250570932667 | 0.1793987366749011 |

Type B isomerisation, configuration P4 of the product

| | | |
|----------------------------|------------|------------|
| 1 | | |
| -7.923688 | -0.000017 | 9.876322 |
| 3.961561 | -6.862259 | 9.876106 |
| 3.961547 | 6.862198 | 9.876070 |
| Si | Al | O |
| 23 | 1 | 48 |
| | 15 | 7 |
| Direct configuration= 2721 | | |
| 0.12112997 | 0.74504799 | 0.27872457 |
| 0.61954427 | 0.23378851 | 0.78138412 |
| 0.85176128 | 0.46743743 | 0.31545840 |
| 0.34394530 | 0.97191474 | 0.82635150 |
| 0.88740654 | 0.19821045 | 0.04648342 |
| 0.40233777 | 0.68879037 | 0.55642147 |
| 0.74725626 | 0.36587030 | 0.21025996 |

| | | |
|------------|------------|------------|
| 0.24221041 | 0.85872866 | 0.71624127 |
| 0.01627324 | 0.63476949 | 0.17684666 |
| 0.51186458 | 0.13657581 | 0.66837285 |
| 0.29001513 | 0.59258033 | 0.44696635 |
| 0.78481067 | 0.08663089 | 0.94584656 |
| 0.28218840 | 0.36789715 | 0.67515382 |
| 0.78637058 | 0.86382248 | 0.17476411 |
| 0.73548555 | 0.14190475 | 0.44001987 |
| 0.24359748 | 0.63400117 | 0.94461056 |
| 0.39223023 | 0.46434861 | 0.78485504 |
| 0.89365115 | 0.97380850 | 0.27617282 |
| 0.12125184 | 0.19748532 | 0.81822730 |
| 0.61910167 | 0.70107894 | 0.31765994 |
| 0.34827836 | 0.74492069 | 0.04802331 |
| 0.84206707 | 0.24651125 | 0.54987575 |
| 0.51463075 | 0.59774919 | 0.21642226 |
| 0.01955557 | 0.08688499 | 0.70951815 |
| 0.22767446 | 0.78353498 | 0.15641578 |
| 0.72790238 | 0.27912866 | 0.66564498 |
| 0.23122642 | 0.08408110 | 0.86782251 |
| 0.73222456 | 0.58069004 | 0.33567816 |
| 0.93144087 | 0.08395128 | 0.15791111 |
| 0.43854745 | 0.57078802 | 0.66715262 |
| 0.70020999 | 0.25895944 | 0.32733733 |
| 0.20544066 | 0.74386957 | 0.83035670 |
| 0.40190198 | 0.25864252 | 0.63669926 |
| 0.90317813 | 0.74990434 | 0.14190582 |
| 0.41060501 | 0.55204359 | 0.33883265 |
| 0.90223572 | 0.05452668 | 0.83799466 |
| 0.17438034 | 0.67330511 | 0.39437722 |
| 0.66189187 | 0.15766928 | 0.90271629 |
| 0.46269908 | 0.01857157 | 0.73936906 |
| 0.97326840 | 0.51221838 | 0.25050726 |
| 0.81367323 | 0.32031392 | 0.09032212 |
| 0.33852717 | 0.80961903 | 0.60002733 |
| 0.46377619 | 0.66304270 | 0.09990186 |
| 0.96852958 | 0.17449134 | 0.58091663 |
| 0.16426287 | 0.32061073 | 0.75221114 |
| 0.66484755 | 0.82069232 | 0.25502676 |
| 0.81632606 | 0.02194884 | 0.39471833 |
| 0.32003269 | 0.50959513 | 0.90580234 |
| 0.01562243 | 0.86771115 | 0.30264987 |
| 0.50862690 | 0.35135854 | 0.81083829 |
| 0.85950334 | 0.37312739 | 0.44657609 |
| 0.37704658 | 0.86749769 | 0.94672576 |
| 0.00667318 | 0.22109976 | 0.93624192 |
| 0.52496035 | 0.70826126 | 0.44929633 |
| 0.62998627 | 0.48206583 | 0.19112592 |
| 0.12712786 | 0.95659777 | 0.67644060 |
| 0.12278544 | 0.61153624 | 0.05481992 |
| 0.61033030 | 0.11742962 | 0.54034590 |
| 0.25956720 | 0.47098750 | 0.54987535 |
| 0.75987786 | 0.96363726 | 0.05223573 |
| 0.06764697 | 0.65677207 | 0.26279682 |
| 0.57304231 | 0.15006940 | 0.75067489 |
| 0.84477830 | 0.40274498 | 0.23173762 |
| 0.31360391 | 0.91476369 | 0.75269286 |
| 0.79578831 | 0.17147380 | 0.00779213 |

| | | |
|------------|------------|------------|
| 0.31313781 | 0.67161632 | 0.50507162 |
| 0.09104683 | 0.17091652 | 0.72274211 |
| 0.55366830 | 0.69627915 | 0.23333207 |
| 0.30178124 | 0.42410739 | 0.75779140 |
| 0.81062628 | 0.91937149 | 0.25484485 |
| 0.32750468 | 0.66415413 | 0.99065195 |
| 0.81283363 | 0.16737076 | 0.49682362 |
| 0.08584487 | 0.24437656 | 0.47874667 |
| 0.21867874 | 0.19501661 | 0.13178120 |
| 0.10737820 | 0.26701026 | 0.24265138 |
| 0.23989168 | 0.31541090 | 0.15168949 |
| 0.11757620 | 0.06672305 | 0.41195522 |
| 0.21912631 | 0.00030979 | 0.29187139 |
| 0.26098412 | 0.96109076 | 0.42564542 |
| 0.17443190 | 0.32020242 | 0.48161720 |
| 0.28839575 | 0.12042494 | 0.56286038 |
| 0.41080800 | 0.15640092 | 0.43576505 |
| 0.38202561 | 0.01736808 | 0.47067352 |
| 0.41033553 | 0.05202606 | 0.15863353 |
| 0.45810696 | 0.01504615 | 0.28638990 |
| 0.45310697 | 0.16026050 | 0.17545975 |
| 0.13109902 | 0.35874143 | 0.34437902 |
| 0.20538624 | 0.23593392 | 0.19957421 |
| 0.21323337 | 0.03456551 | 0.36178248 |
| 0.27306012 | 0.14085744 | 0.29134444 |
| 0.25973993 | 0.18344608 | 0.39058491 |
| 0.16419307 | 0.28752892 | 0.41942245 |
| 0.33827960 | 0.11232339 | 0.47048888 |
| 0.40738110 | 0.08881961 | 0.22509219 |

Type B isomerisation, configuration R5 of the reactant

| | | | | |
|-----------|-----------|----------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |

Direct configuration= 1579

| | | |
|------------|------------|------------|
| 0.12751633 | 0.74446553 | 0.28835514 |
| 0.62680462 | 0.23816731 | 0.78977916 |
| 0.85954257 | 0.46735124 | 0.32276818 |
| 0.35501970 | 0.97119695 | 0.83461558 |
| 0.90130710 | 0.19680709 | 0.05671525 |
| 0.40860112 | 0.68988841 | 0.56169669 |
| 0.75288837 | 0.36403328 | 0.22144671 |
| 0.25238043 | 0.86171613 | 0.72218060 |
| 0.02101014 | 0.63805452 | 0.18158840 |
| 0.52016153 | 0.13707301 | 0.68245666 |
| 0.29715510 | 0.59506541 | 0.45576403 |
| 0.79966019 | 0.08355507 | 0.95061692 |
| 0.29167703 | 0.36502451 | 0.68714243 |
| 0.79200122 | 0.86522286 | 0.18372752 |
| 0.74611967 | 0.14210445 | 0.44960355 |
| 0.24809067 | 0.63940839 | 0.95088854 |
| 0.39934550 | 0.46297959 | 0.79435810 |
| 0.90074516 | 0.97148739 | 0.28857227 |
| 0.12803345 | 0.19774962 | 0.83305897 |
| 0.62585923 | 0.70125136 | 0.32500654 |

| | | |
|------------|------------|------------|
| 0.35451890 | 0.74554757 | 0.05831934 |
| 0.85147305 | 0.24824984 | 0.55594718 |
| 0.52117763 | 0.59766964 | 0.22596099 |
| 0.02547388 | 0.08442356 | 0.72027861 |
| 0.23540681 | 0.78496507 | 0.16795944 |
| 0.72707165 | 0.28180173 | 0.66412657 |
| 0.24323634 | 0.08499821 | 0.87620185 |
| 0.73915189 | 0.58030952 | 0.33874414 |
| 0.93904139 | 0.08249833 | 0.17129794 |
| 0.43883869 | 0.56498192 | 0.66872114 |
| 0.70478411 | 0.25782043 | 0.33829944 |
| 0.20863286 | 0.75110517 | 0.83864760 |
| 0.41052700 | 0.25695166 | 0.64530971 |
| 0.90781518 | 0.75257699 | 0.14552856 |
| 0.41786783 | 0.55185650 | 0.34895225 |
| 0.91305815 | 0.03468031 | 0.84797074 |
| 0.18016376 | 0.66673353 | 0.40408685 |
| 0.67880676 | 0.16468546 | 0.90512997 |
| 0.47452258 | 0.01664415 | 0.75060344 |
| 0.97971187 | 0.51450012 | 0.25404363 |
| 0.81877245 | 0.31766237 | 0.10166375 |
| 0.35147302 | 0.80516313 | 0.61231057 |
| 0.47017192 | 0.66087105 | 0.10937531 |
| 0.97002065 | 0.17615036 | 0.59770323 |
| 0.17199370 | 0.31991304 | 0.75767818 |
| 0.67141799 | 0.82077679 | 0.26405937 |
| 0.82104106 | 0.02023470 | 0.40623900 |
| 0.32620943 | 0.51639087 | 0.90996167 |
| 0.02427159 | 0.86767916 | 0.31531471 |
| 0.51935161 | 0.35704635 | 0.82259809 |
| 0.86896616 | 0.37625713 | 0.45417825 |
| 0.38406505 | 0.86854114 | 0.95796680 |
| 0.02681021 | 0.22292226 | 0.95928422 |
| 0.53467948 | 0.70405694 | 0.45850798 |
| 0.63795588 | 0.48261461 | 0.20128938 |
| 0.14179062 | 0.96237258 | 0.67636037 |
| 0.12789845 | 0.61334717 | 0.06011138 |
| 0.62623110 | 0.11800760 | 0.55893314 |
| 0.27140569 | 0.47654614 | 0.56666856 |
| 0.76090701 | 0.97113440 | 0.06588582 |
| 0.07148219 | 0.66282299 | 0.26627135 |
| 0.56873149 | 0.15356924 | 0.77379920 |
| 0.85382371 | 0.39793931 | 0.24170491 |
| 0.32386873 | 0.91506738 | 0.76158640 |
| 0.82489219 | 0.16842293 | 0.00178432 |
| 0.31730393 | 0.68558581 | 0.50302108 |
| 0.08179487 | 0.16684829 | 0.75430592 |
| 0.55812413 | 0.69895567 | 0.24099085 |
| 0.31082159 | 0.40759571 | 0.78191553 |
| 0.82167755 | 0.91443320 | 0.26541120 |
| 0.33038849 | 0.66825185 | 0.00003201 |
| 0.83371773 | 0.16976083 | 0.49204216 |
| 0.24165076 | 0.20662513 | 0.44390757 |
| 0.20921903 | 0.33576796 | 0.01313738 |
| 0.05835235 | 0.32600101 | 0.10739292 |
| 0.14525060 | 0.34938102 | 0.16617697 |
| 0.15478638 | 0.06075183 | 0.45938643 |
| 0.04325435 | 0.17163119 | 0.31810844 |

| | | |
|------------|------------|------------|
| 0.13853574 | 0.02333811 | 0.29899996 |
| 0.27266687 | 0.26344729 | 0.28365400 |
| 0.37424423 | 0.99061313 | 0.41999826 |
| 0.40111639 | 0.05053136 | 0.26040692 |
| 0.33698308 | 0.92688912 | 0.34380242 |
| 0.26016653 | 0.09419407 | 0.02328686 |
| 0.33315751 | 0.00344574 | 0.13987935 |
| 0.36872774 | 0.14212377 | 0.02812369 |
| 0.11913401 | 0.28651899 | 0.38100047 |
| 0.15369108 | 0.30187676 | 0.10540743 |
| 0.13598619 | 0.11608799 | 0.28475641 |
| 0.19538309 | 0.17104369 | 0.15977835 |
| 0.21110739 | 0.10099078 | 0.36955965 |
| 0.21066906 | 0.22204973 | 0.36785997 |
| 0.33792159 | 0.01268015 | 0.34569188 |
| 0.29756781 | 0.09709499 | 0.08826508 |

Type B isomerisation, configuration TS5 of the TS

| | | |
|---------------------|---------------------|--------------------|
| 1.0000000000000000 | | |
| -7.9236880000000000 | -0.0000170000000000 | 9.8763220000000000 |
| 3.9615610000000000 | -6.8622589999999999 | 9.8761060000000001 |
| 3.9615469999999999 | 6.8621980000000002 | 9.8760700000000003 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1251136474933943 | 0.7493755337758820 | 0.2839360634635866 |
| 0.6276960276804560 | 0.2422958532541487 | 0.7830515086027636 |
| 0.8624726777963382 | 0.4683482393089715 | 0.3168926362480446 |
| 0.3497473850392512 | 0.9800543774619030 | 0.8314404032617607 |
| 0.8959709301876491 | 0.2040671289535347 | 0.0492525376988009 |
| 0.4097779655949729 | 0.6934198218809232 | 0.5595147328801344 |
| 0.7508787608944676 | 0.3702196885943281 | 0.2145334976208155 |
| 0.2532779324450953 | 0.8645469091217181 | 0.7190818173416739 |
| 0.0217499290113518 | 0.6406192026665866 | 0.1804800068118893 |
| 0.5178924141377996 | 0.1436721087057596 | 0.6724444781798955 |
| 0.2964332129760016 | 0.6025230046155103 | 0.4504772986010361 |
| 0.7953008095242120 | 0.0860224694056278 | 0.9478534126786129 |
| 0.2885617536574048 | 0.3717143063303049 | 0.6812879783821038 |
| 0.7928522500223678 | 0.8679159971821373 | 0.1794713544889810 |
| 0.7401443583960579 | 0.1476630051773966 | 0.4432947254116197 |
| 0.2526775002000245 | 0.6408654534395208 | 0.9478506623786804 |
| 0.3957436233545956 | 0.4651880607460642 | 0.7931744045515376 |
| 0.9012869780123319 | 0.9798327203931656 | 0.2795137010235971 |
| 0.1246964602814483 | 0.2045527706933445 | 0.8235575578329541 |
| 0.6292173185281690 | 0.7012391798554164 | 0.3254385138895902 |
| 0.3552987732292905 | 0.7505427393520809 | 0.0516264618084181 |
| 0.8498252955602570 | 0.2508946274848662 | 0.5524359954061757 |
| 0.5205184851472600 | 0.6043949101206808 | 0.2219538387024524 |
| 0.0245502460300218 | 0.0868175519173026 | 0.7153935915424569 |
| 0.2323097759291645 | 0.7833892310874849 | 0.1604515734422955 |
| 0.7331987085585757 | 0.2891722825012083 | 0.6644768379479890 |
| 0.2367625955193871 | 0.0925492167676531 | 0.8712607624590437 |
| 0.7423740640900173 | 0.5809308820213196 | 0.3378066575064270 |
| 0.9390388611984443 | 0.0911032179630168 | 0.1625760481729116 |
| 0.4330304755634893 | 0.5719045521166302 | 0.6705695704387820 |
| 0.7023758867410982 | 0.2638778105668459 | 0.3311339212245185 |
| 0.2142773300902099 | 0.7509826019812168 | 0.8333898486904547 |
| 0.4084412854590571 | 0.2650588920254279 | 0.6377926280980221 |

| | | |
|--------------------|--------------------|--------------------|
| 0.9090815518424706 | 0.7552408982118985 | 0.1427998197034590 |
| 0.4154188658463461 | 0.5585718914107667 | 0.3430632407230912 |
| 0.9115634169998303 | 0.0414165043532222 | 0.8443960830647306 |
| 0.1792186962643256 | 0.6795054007266635 | 0.3993417793831177 |
| 0.6746222688225529 | 0.1639193102677349 | 0.9014866452331405 |
| 0.4694766019267819 | 0.0252775673012576 | 0.7472868531146913 |
| 0.9819118235713545 | 0.5163976245530044 | 0.2475444756239644 |
| 0.8137877066474865 | 0.3247490914692082 | 0.0944905405285507 |
| 0.3511357408267738 | 0.8136533030027259 | 0.6039609993672621 |
| 0.4702967486122704 | 0.6729274751218224 | 0.1049145856993284 |
| 0.9714157019046060 | 0.1697906601686153 | 0.5890616464036016 |
| 0.1690461987782625 | 0.3266843722015774 | 0.7481168360200979 |
| 0.6739161304827074 | 0.8214077192034024 | 0.2649472633334500 |
| 0.8225089693888853 | 0.0273531184193072 | 0.3982155454622808 |
| 0.3248055606697307 | 0.5154514751268727 | 0.9108368668368076 |
| 0.0247028561950519 | 0.8756139812365800 | 0.3063732749875119 |
| 0.5177466744920710 | 0.3594649958888529 | 0.8160514482645055 |
| 0.8732655215308915 | 0.3752883035401501 | 0.4477730448529477 |
| 0.3793130231108652 | 0.8763166098494788 | 0.9538872835304648 |
| 0.0168106475798685 | 0.2324460706584453 | 0.9450353576502403 |
| 0.5391751994428643 | 0.7020881428746023 | 0.4602382194007127 |
| 0.6355982816748000 | 0.4890739307109530 | 0.1957500480732470 |
| 0.1405373113048463 | 0.9621949383632725 | 0.6732180021478895 |
| 0.1323161011237800 | 0.6223112445615985 | 0.0596279670245435 |
| 0.6177445944519132 | 0.1205437939697963 | 0.5465406256963874 |
| 0.2687498014516324 | 0.4851548028940911 | 0.5612663920585663 |
| 0.7595402559942341 | 0.9701958648068413 | 0.0605812356517327 |
| 0.0653103644863461 | 0.6644014647710280 | 0.2718491459673601 |
| 0.5776574201472379 | 0.1604109990475318 | 0.7539240250613617 |
| 0.8512893670587693 | 0.4033146987684395 | 0.2357338676329867 |
| 0.3218222973613135 | 0.9219964348417826 | 0.7566389411277840 |
| 0.8150019581901780 | 0.1709846707261639 | 1.0032480368268215 |
| 0.3199221109328558 | 0.6922944806964798 | 0.4966005622694399 |
| 0.0841268151495090 | 0.1728330704985217 | 0.7399628714128377 |
| 0.5587489085810677 | 0.7015106089586235 | 0.2424783660365752 |
| 0.3072060454148797 | 0.4137173903963111 | 0.7764313171944947 |
| 0.8218234858974270 | 0.9230095922588846 | 0.2565909666616572 |
| 0.3413222854564529 | 0.6693387103074581 | 0.9896468643486872 |
| 0.8192436212336962 | 0.1753299016301721 | 0.4960168433734848 |
| 0.3202452835345506 | 0.1218899452144932 | 0.4726662668048057 |
| 0.1824633689390163 | 0.2771874832749704 | 0.1925717079004859 |
| 0.0559801113042078 | 0.2370968341921865 | 0.2108670808463839 |
| 0.0706915060932044 | 0.2543902353113623 | 0.3365139456157929 |
| 0.2391835476668221 | 0.9852131280996758 | 0.4698157241711204 |
| 0.0702910587259443 | 0.0464877498694294 | 0.4746044610028658 |
| 0.1696435436247398 | 0.9123075153086367 | 0.4157087148025872 |
| 0.2926274055529051 | 0.2273060323817634 | 0.3331880137297777 |
| 0.4546986936212455 | 0.9502572854831064 | 0.3885967742709543 |
| 0.4463248758692446 | 0.0327984436094323 | 0.2372571530045191 |
| 0.4055276767921820 | 0.8958137303134751 | 0.3128648941580840 |
| 0.1856324558369393 | 0.0652022353030794 | 0.1319944388322360 |
| 0.2936675257397009 | 0.9430987463113640 | 0.2010268247246901 |
| 0.3240688332440487 | 0.0851202916016246 | 0.1125643800656876 |
| 0.1686587708367805 | 0.1947051370911308 | 0.4644248432962891 |
| 0.1206510851094483 | 0.2223208676996101 | 0.2561435692742691 |
| 0.1454439390396617 | 0.0093130682661244 | 0.4038486092781588 |
| 0.1900025012880333 | 0.0891049193482654 | 0.2871968066051648 |
| 0.2741238999201785 | 0.0511893951905934 | 0.3754887724697561 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2619859890276540 | 0.1561154797531477 | 0.4138992068184287 |
| 0.4029710286917891 | 0.9774240542957388 | 0.3256211574724927 |
| 0.2531694097361875 | 0.0417136181643269 | 0.1776378929646742 |

Type B isomerisation, configuration P5 of the product

| | | | | |
|-----------|-----------|----------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |

Direct configuration= 2816

| | | |
|------------|------------|------------|
| 0.12568489 | 0.74437478 | 0.28147496 |
| 0.62397418 | 0.23347889 | 0.78435203 |
| 0.85640385 | 0.46675392 | 0.31820102 |
| 0.34859766 | 0.97127953 | 0.82904385 |
| 0.89204321 | 0.19796094 | 0.04915983 |
| 0.40701204 | 0.68809870 | 0.55921654 |
| 0.75174464 | 0.36514221 | 0.21325460 |
| 0.24712194 | 0.85834304 | 0.71852664 |
| 0.02050840 | 0.63454159 | 0.17964950 |
| 0.51663536 | 0.13598109 | 0.67120216 |
| 0.29470073 | 0.59201179 | 0.44955030 |
| 0.78929602 | 0.08615178 | 0.94859562 |
| 0.28688819 | 0.36726232 | 0.67772302 |
| 0.79045224 | 0.86368475 | 0.17814462 |
| 0.73976625 | 0.14179157 | 0.44261344 |
| 0.24794631 | 0.63372761 | 0.94714963 |
| 0.39631295 | 0.46379353 | 0.78792403 |
| 0.89818459 | 0.97348196 | 0.27910664 |
| 0.12557094 | 0.19697966 | 0.82108663 |
| 0.62345263 | 0.70067965 | 0.32024995 |
| 0.35297409 | 0.74414352 | 0.05061992 |
| 0.84622875 | 0.24685075 | 0.55273494 |
| 0.51917451 | 0.59754968 | 0.21905136 |
| 0.02363629 | 0.08628489 | 0.71231701 |
| 0.23238012 | 0.78245096 | 0.15913962 |
| 0.73231807 | 0.27910597 | 0.66883875 |
| 0.23559163 | 0.08334309 | 0.87033340 |
| 0.73681546 | 0.58028508 | 0.33681839 |
| 0.93574461 | 0.08360863 | 0.16069638 |
| 0.44253958 | 0.57042042 | 0.67046737 |
| 0.70381575 | 0.25822839 | 0.32971217 |
| 0.21035293 | 0.74340509 | 0.83253290 |
| 0.40677327 | 0.25810462 | 0.63934921 |
| 0.90723001 | 0.74975031 | 0.14533645 |
| 0.41516486 | 0.55149818 | 0.34129922 |
| 0.90637053 | 0.05332326 | 0.84070335 |
| 0.17893289 | 0.67279155 | 0.39715452 |
| 0.66617258 | 0.15734379 | 0.90577908 |
| 0.46733275 | 0.01808270 | 0.74244395 |
| 0.97781458 | 0.51176415 | 0.25270918 |
| 0.81799019 | 0.32005728 | 0.09301633 |
| 0.34330234 | 0.80934341 | 0.60216846 |
| 0.46860765 | 0.66223764 | 0.10233853 |
| 0.97266803 | 0.17395915 | 0.58368092 |
| 0.16904883 | 0.31983437 | 0.75445815 |
| 0.66896959 | 0.82042113 | 0.25825409 |

| | | |
|------------|------------|------------|
| 0.82157339 | 0.02170547 | 0.39768160 |
| 0.32381166 | 0.50894361 | 0.90892758 |
| 0.02028513 | 0.86722524 | 0.30504806 |
| 0.51275231 | 0.35084733 | 0.81388448 |
| 0.86380520 | 0.37379689 | 0.44999608 |
| 0.38151728 | 0.86689366 | 0.94950971 |
| 0.01157151 | 0.22097724 | 0.93937429 |
| 0.53017524 | 0.70655832 | 0.45252244 |
| 0.63512867 | 0.48217993 | 0.19410341 |
| 0.13201491 | 0.95643211 | 0.67893709 |
| 0.12681373 | 0.61213120 | 0.05725374 |
| 0.61501790 | 0.11651556 | 0.54323700 |
| 0.26437838 | 0.47032851 | 0.55240140 |
| 0.76412285 | 0.96355419 | 0.05557952 |
| 0.07201227 | 0.65603109 | 0.26586082 |
| 0.57795013 | 0.14964310 | 0.75326079 |
| 0.84981625 | 0.40037569 | 0.23573754 |
| 0.31876630 | 0.91405489 | 0.75505391 |
| 0.80096839 | 0.17131180 | 0.00967849 |
| 0.31798497 | 0.67093126 | 0.50764499 |
| 0.09431779 | 0.17066761 | 0.72616875 |
| 0.55719659 | 0.69674312 | 0.23611574 |
| 0.30608400 | 0.42352824 | 0.76056557 |
| 0.81455446 | 0.91924543 | 0.25835440 |
| 0.33224659 | 0.66355054 | 0.99300890 |
| 0.81630115 | 0.16890621 | 0.49892766 |
| 0.17756132 | 0.32147970 | 0.48628446 |
| 0.24617360 | 0.31781090 | 0.15494342 |
| 0.22599208 | 0.19739630 | 0.13408266 |
| 0.11376077 | 0.26900561 | 0.24488730 |
| 0.12386599 | 0.06816430 | 0.41381828 |
| 0.22651192 | 0.00234169 | 0.29356997 |
| 0.26730958 | 0.96292778 | 0.42801952 |
| 0.13545046 | 0.36032189 | 0.34827029 |
| 0.29123742 | 0.12125613 | 0.56763209 |
| 0.41390136 | 0.15885701 | 0.44191285 |
| 0.38700189 | 0.01941105 | 0.47445748 |
| 0.41759535 | 0.05524043 | 0.16148174 |
| 0.46413160 | 0.01750678 | 0.29021055 |
| 0.45928373 | 0.16316613 | 0.18008343 |
| 0.09004118 | 0.24546736 | 0.48201314 |
| 0.21189987 | 0.23818402 | 0.20229268 |
| 0.21975004 | 0.03641581 | 0.36400721 |
| 0.27911271 | 0.14310454 | 0.29442736 |
| 0.26443214 | 0.18526587 | 0.39446819 |
| 0.16811588 | 0.28894868 | 0.42348873 |
| 0.34221726 | 0.11407176 | 0.47508059 |
| 0.41376936 | 0.09155166 | 0.22873822 |

Type B isomerisation, configuration R6 of the reactant

1

| | | |
|-----------|-----------|----------|
| -7.923688 | -0.000017 | 9.876322 |
| 3.961561 | -6.862259 | 9.876106 |
| 3.961547 | 6.862198 | 9.876070 |

Si Al O H C

23 1 48 15 7

Direct configuration= 904

| | | |
|------------|------------|------------|
| 0.12164134 | 0.75106276 | 0.28620970 |
|------------|------------|------------|

| | | |
|------------|------------|------------|
| 0.62422020 | 0.24158775 | 0.78520442 |
| 0.85671240 | 0.47033713 | 0.32034308 |
| 0.34565406 | 0.98000927 | 0.83381948 |
| 0.89044674 | 0.20486138 | 0.05241626 |
| 0.40541367 | 0.69598829 | 0.56127841 |
| 0.74792842 | 0.37144792 | 0.21686504 |
| 0.24743295 | 0.86458746 | 0.72274132 |
| 0.01878821 | 0.64073116 | 0.18190071 |
| 0.51347003 | 0.14418876 | 0.67528748 |
| 0.29213663 | 0.60222290 | 0.45310980 |
| 0.78973070 | 0.08941114 | 0.95023319 |
| 0.28426685 | 0.37375296 | 0.68424023 |
| 0.78996752 | 0.86861866 | 0.17892750 |
| 0.73581520 | 0.14859183 | 0.44539106 |
| 0.24854230 | 0.64058900 | 0.95050496 |
| 0.39452722 | 0.46821700 | 0.79293273 |
| 0.89582184 | 0.98010596 | 0.28225423 |
| 0.12166156 | 0.20514785 | 0.82525774 |
| 0.62366450 | 0.70434314 | 0.32589345 |
| 0.35053379 | 0.75229679 | 0.05500164 |
| 0.84765344 | 0.25014746 | 0.55382694 |
| 0.51621407 | 0.60477775 | 0.22424443 |
| 0.02162320 | 0.09108350 | 0.71497375 |
| 0.22907869 | 0.78857654 | 0.16398758 |
| 0.73131413 | 0.28575997 | 0.66755726 |
| 0.23287694 | 0.09254594 | 0.87471524 |
| 0.73548848 | 0.58250991 | 0.34043586 |
| 0.93481963 | 0.09211667 | 0.16589027 |
| 0.43446442 | 0.57418996 | 0.67089600 |
| 0.69894116 | 0.26499416 | 0.33275106 |
| 0.20977460 | 0.74958619 | 0.83617418 |
| 0.40379246 | 0.26599578 | 0.64253380 |
| 0.90652665 | 0.75563587 | 0.14370027 |
| 0.41151111 | 0.55856609 | 0.34536738 |
| 0.90646076 | 0.05167473 | 0.84455613 |
| 0.17519185 | 0.67892294 | 0.40166737 |
| 0.66761866 | 0.16519990 | 0.90605387 |
| 0.46494290 | 0.02574413 | 0.74862050 |
| 0.97631594 | 0.51805762 | 0.25233327 |
| 0.81170634 | 0.32652350 | 0.09639517 |
| 0.34494664 | 0.81508875 | 0.60706180 |
| 0.46612344 | 0.67226905 | 0.10706329 |
| 0.97064878 | 0.17246178 | 0.58765718 |
| 0.16519780 | 0.32794320 | 0.75578321 |
| 0.67010835 | 0.82347551 | 0.26289695 |
| 0.81531358 | 0.02782917 | 0.40044820 |
| 0.32543672 | 0.51609027 | 0.91222747 |
| 0.01916310 | 0.87623636 | 0.30913170 |
| 0.51491016 | 0.35991284 | 0.81565344 |
| 0.86713628 | 0.37673097 | 0.45071755 |
| 0.37631658 | 0.87775519 | 0.95704930 |
| 0.01140191 | 0.23023617 | 0.94655147 |
| 0.53194897 | 0.71087704 | 0.45865302 |
| 0.63273336 | 0.49044227 | 0.19813351 |
| 0.13314360 | 0.96195784 | 0.68146692 |
| 0.12851555 | 0.61832091 | 0.06158081 |
| 0.61255990 | 0.12330864 | 0.54838222 |
| 0.26376825 | 0.48391591 | 0.56241420 |

| | | |
|------------|------------|------------|
| 0.75815138 | 0.96975065 | 0.05904900 |
| 0.06476614 | 0.66606065 | 0.27018524 |
| 0.57369719 | 0.15865825 | 0.75790802 |
| 0.84881212 | 0.40387964 | 0.23822829 |
| 0.31719421 | 0.91992728 | 0.76180360 |
| 0.80533994 | 0.17241290 | 0.01118139 |
| 0.31657970 | 0.68945627 | 0.50107633 |
| 0.08539291 | 0.17606703 | 0.73663465 |
| 0.55306669 | 0.70373469 | 0.24348095 |
| 0.30354189 | 0.42019787 | 0.77558118 |
| 0.81763284 | 0.92452596 | 0.25628413 |
| 0.33297456 | 0.67236303 | 0.99464670 |
| 0.81624623 | 0.17531515 | 0.49716480 |
| 0.25460780 | 0.29842258 | 0.38973400 |
| 0.19193800 | 0.20728922 | 0.09786780 |
| 0.08432728 | 0.12784617 | 0.19106727 |
| 0.08843439 | 0.23747917 | 0.24141846 |
| 0.24226791 | 0.09014259 | 0.50303864 |
| 0.10858366 | 0.07845630 | 0.43369265 |
| 0.24356081 | 0.94758574 | 0.43223643 |
| 0.24657843 | 0.28903699 | 0.25726869 |
| 0.44451483 | 0.10379254 | 0.25859129 |
| 0.44394022 | 0.97458693 | 0.39071460 |
| 0.44654140 | 0.11256848 | 0.39350398 |
| 0.40485016 | 0.04288980 | 0.14807792 |
| 0.32116533 | 0.98821749 | 0.11161621 |
| 0.37562529 | 0.90278995 | 0.24485522 |
| 0.12009572 | 0.28363098 | 0.39250939 |
| 0.14616880 | 0.16859697 | 0.19370666 |
| 0.20459052 | 0.04280770 | 0.38605530 |
| 0.22775253 | 0.06652123 | 0.25853319 |
| 0.27157234 | 0.11838249 | 0.40315160 |
| 0.21951167 | 0.25493553 | 0.35702076 |
| 0.40902739 | 0.07380924 | 0.35819460 |
| 0.33608769 | 0.99279591 | 0.18927441 |

Type B isomerisation, configuration TS6 of the TS

| | | |
|---------------------|---------------------|--------------------|
| 1.0000000000000000 | | |
| -7.9236880000000003 | -0.0000170000000000 | 9.8763220000000000 |
| 3.9615610000000001 | -6.8622589999999999 | 9.8761060000000001 |
| 3.9615469999999999 | 6.8621980000000002 | 9.8760700000000003 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1216184117560316 | 0.7514092261116713 | 0.2853346774328333 |
| 0.6262556183550545 | 0.2462875446776689 | 0.7809415534876550 |
| 0.8595060556621540 | 0.4701101899778354 | 0.3188552197509849 |
| 0.3485926624801768 | 0.9818514417209271 | 0.8325313960910782 |
| 0.8933221563301040 | 0.2049770830731315 | 0.0509896884808218 |
| 0.4076600610648039 | 0.6936289977899575 | 0.5602638082928206 |
| 0.7474479020167000 | 0.3719940195358585 | 0.2147604930698177 |
| 0.2521709595439837 | 0.8672201564637639 | 0.7205450268762019 |
| 0.0193955085439390 | 0.6428946332252252 | 0.1797375162196854 |
| 0.5148834077784569 | 0.1460572773505157 | 0.6733601762740489 |
| 0.2932222999571791 | 0.6035829888011101 | 0.4518961699691742 |
| 0.7967877860654483 | 0.0867959523226679 | 0.9484210305915297 |
| 0.2860009483478184 | 0.3740623699392776 | 0.6829894197767300 |
| 0.7909439313426676 | 0.8698471745973542 | 0.1779907672839510 |

| | | |
|--------------------|--------------------|---------------------|
| 0.7359607582222955 | 0.1494562145461165 | 0.4430966458280126 |
| 0.2484148929113291 | 0.6462947476475518 | 0.9475562774249947 |
| 0.3968112673893730 | 0.4676600768607308 | 0.7919767431487597 |
| 0.8976393618842106 | 0.9808310315205199 | 0.2808862890052785 |
| 0.1222304302287409 | 0.2080965419612571 | 0.8230712145843024 |
| 0.6276413976352262 | 0.7022579972720605 | 0.3254007789957690 |
| 0.3507727474062577 | 0.7546794192683930 | 0.0535746991312407 |
| 0.8453244987331739 | 0.2525692701301316 | 0.5525269388947106 |
| 0.5180367518982781 | 0.6049925543397945 | 0.2222784243796104 |
| 0.0237813005634545 | 0.0905546652296162 | 0.7171411887530801 |
| 0.2277954426630654 | 0.7883201829859701 | 0.1619761707236385 |
| 0.7251770091802971 | 0.2990812969457661 | 0.6580720790090319 |
| 0.2342255744944630 | 0.0946742870018984 | 0.8691277766990503 |
| 0.7382947397554660 | 0.5803121221434733 | 0.3471949604780086 |
| 0.9362478646627724 | 0.0920012136456544 | 0.1643162322293812 |
| 0.4395333344869535 | 0.5690010695357982 | 0.6658879214112565 |
| 0.6989536206425062 | 0.2650293065571232 | 0.3303364875224669 |
| 0.2047083663820742 | 0.7594201366656123 | 0.8371187965865891 |
| 0.4037547277471392 | 0.2657540434122161 | 0.6398255049595983 |
| 0.9080947069943752 | 0.7582621420926967 | 0.1402209071684875 |
| 0.4135611111969252 | 0.5606917866307575 | 0.3450309892996683 |
| 0.9197362615080609 | 0.0388070388469719 | 0.8522482730721970 |
| 0.1765655564161353 | 0.6793325853251693 | 0.4000784725587334 |
| 0.6822183608500620 | 0.1646726213769061 | 0.8928719724422832 |
| 0.4686865414443460 | 0.0265174128021384 | 0.7497054118676422 |
| 0.9775829612591729 | 0.5199353407010302 | 0.2472121932724304 |
| 0.8137780391876663 | 0.3266839984686939 | 0.0946586625705516 |
| 0.3482344276075063 | 0.8100367964947991 | 0.6100039235087189 |
| 0.4654108344071893 | 0.6749619775145752 | 0.1069248632089442 |
| 0.9607818725744963 | 0.1669325647562417 | 0.5979970884571033 |
| 0.1654368816836372 | 0.3309562472404160 | 0.7533633893562419 |
| 0.6730828355737425 | 0.8218460339617979 | 0.2630637146185591 |
| 0.8170736308394957 | 0.0283420640416129 | 0.3993913381281547 |
| 0.3242295165105204 | 0.5241888347770708 | 0.9052013707840515 |
| 0.0199229375253835 | 0.8762159154937398 | 0.3098488654904583 |
| 0.5156841780057297 | 0.3599502833929862 | 0.8214964295005610 |
| 0.8790770323994135 | 0.3719969821577662 | 0.4454516216274721 |
| 0.3759630723157213 | 0.8803550612475293 | 0.9567493326238186 |
| 0.0140198743521220 | 0.2314111041533862 | 0.9455997333043765 |
| 0.5320162961260109 | 0.7113801543947187 | 0.4560673730001360 |
| 0.6308857459248728 | 0.4887448849606364 | 0.1945276913733050 |
| 0.1445018059449743 | 0.9707419087184614 | 0.6689383910167802 |
| 0.1306137591377358 | 0.6213343629865228 | 0.0601539616283677 |
| 0.6133994508510506 | 0.1235338965965749 | 0.5468207020766925 |
| 0.2658192350114318 | 0.4856795729524624 | 0.5620017698640710 |
| 0.7560264619268783 | 0.9726479876677252 | 0.0599249156164122 |
| 0.0631786535119884 | 0.6666166969265966 | 0.2709087505477167 |
| 0.5746785725939020 | 0.1645892566270849 | 0.7534875245317264 |
| 0.8447634270872227 | 0.4077853952872281 | 0.2377297671724166 |
| 0.3243857297665049 | 0.9209102149238837 | 0.7576241028180841 |
| 0.8093365391742358 | 0.1734730596887314 | 0.0071708110959535 |
| 0.3149897659870015 | 0.6924475222888652 | 0.5007038168858619 |
| 0.0828473482210000 | 0.1821173617833322 | 0.7342596673948368 |
| 0.5616629908135736 | 0.6995073018008384 | 0.2403002924938414 |
| 0.3077138427475706 | 0.4167180937942849 | 0.7755831573098761 |
| 0.8192042415808112 | 0.9245700739083049 | 0.2558664792735574 |
| 0.3358811310373879 | 0.6753322604520050 | -0.0097738347253934 |
| 0.8154209563910120 | 0.1778559114766762 | 0.4947291483685895 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2453940727862566 | 0.2126352640292708 | 0.4685969678579067 |
| 0.1670806182757927 | 0.2627494237961838 | 0.1776144365216367 |
| 0.0826213671424974 | 0.1755431979714866 | 0.1857476836479691 |
| 0.0433231283302344 | 0.2319383356923107 | 0.3087510473234065 |
| 0.2136575350246341 | 0.0317011792274411 | 0.4917780197171923 |
| 0.0675739334124770 | 0.0413697990635365 | 0.4702867538922125 |
| 0.2023059465200931 | 0.9079289763926970 | 0.4434805557564736 |
| 0.2456379861740834 | 0.2748787473925671 | 0.3132640398227153 |
| 0.4393171336684705 | 0.0752144900158226 | 0.2788879575265877 |
| 0.4189674972216957 | 0.9307776162868573 | 0.3728804120944073 |
| 0.4191685410259163 | 0.0303505556331042 | 0.4380492727633142 |
| 0.3636838490809436 | 0.0697465856859396 | 0.1363645265872136 |
| 0.2575236376897688 | 0.0053478308708408 | 0.1471093055059893 |
| 0.3562073644814924 | 0.9240956502738966 | 0.2405169966980361 |
| 0.1113957283403048 | 0.2481796401847068 | 0.4320700420316410 |
| 0.1193227142213783 | 0.1943007551530862 | 0.2390462890799471 |
| 0.1586700906035096 | 1.0056035768390823 | 0.4139807985198825 |
| 0.2047331341524368 | 0.0768610149844751 | 0.2930571259640595 |
| 0.2551202870333864 | 0.0854436229038606 | 0.3914368475914613 |
| 0.2103314469911933 | 0.2138185869002447 | 0.4016950704445577 |
| 0.3913165268857472 | 0.0260378796133271 | 0.3687714828294533 |
| 0.3020842416630933 | 0.0146325176254437 | 0.1999197487041638 |

Type B isomerisation, configuration P6 of the product

| | | | | |
|---------------------------|------------|------------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |
| Direct configuration= 567 | | | | |
| 0.12210687 | 0.75217694 | 0.28522581 | | |
| 0.62516020 | 0.24458005 | 0.78072024 | | |
| 0.85830648 | 0.47092312 | 0.32208276 | | |
| 0.34696523 | 0.98137844 | 0.83280337 | | |
| 0.89004430 | 0.20534044 | 0.05153469 | | |
| 0.40695796 | 0.69460389 | 0.56175918 | | |
| 0.74804516 | 0.37261621 | 0.21512274 | | |
| 0.24820452 | 0.86548865 | 0.72353214 | | |
| 0.02001144 | 0.64208325 | 0.18097737 | | |
| 0.51326106 | 0.14571314 | 0.67360317 | | |
| 0.29291071 | 0.60233050 | 0.45296359 | | |
| 0.79433173 | 0.08976505 | 0.95158700 | | |
| 0.28516327 | 0.37418547 | 0.68334854 | | |
| 0.79186193 | 0.86876987 | 0.17697210 | | |
| 0.73746206 | 0.14854675 | 0.44309193 | | |
| 0.24993420 | 0.64259441 | 0.95026759 | | |
| 0.39834546 | 0.46792848 | 0.79176450 | | |
| 0.89733909 | 0.98045857 | 0.28019724 | | |
| 0.12379132 | 0.20641406 | 0.82162638 | | |
| 0.62749489 | 0.70183927 | 0.32802160 | | |
| 0.35151746 | 0.75388902 | 0.05401332 | | |
| 0.84618086 | 0.25012576 | 0.55301328 | | |
| 0.51796900 | 0.60332461 | 0.22383435 | | |
| 0.02508245 | 0.09102483 | 0.71854005 | | |
| 0.22807150 | 0.78911346 | 0.16153232 | | |
| 0.72231719 | 0.29663406 | 0.65569752 | | |
| 0.23385300 | 0.09393899 | 0.87257725 | | |

| | | |
|------------|------------|------------|
| 0.73766814 | 0.58045375 | 0.35421324 |
| 0.93544951 | 0.09179152 | 0.16338114 |
| 0.44173044 | 0.57087037 | 0.66767313 |
| 0.70106621 | 0.26450939 | 0.33021818 |
| 0.20608532 | 0.75485570 | 0.84005503 |
| 0.40230138 | 0.26555824 | 0.63961796 |
| 0.90937314 | 0.75724767 | 0.13950095 |
| 0.41302099 | 0.55888767 | 0.34593839 |
| 0.92227769 | 0.04774535 | 0.85841119 |
| 0.17719709 | 0.68070499 | 0.39982505 |
| 0.68291727 | 0.16305949 | 0.89141538 |
| 0.46679299 | 0.02611783 | 0.74701255 |
| 0.97684722 | 0.51996912 | 0.25056816 |
| 0.81845212 | 0.32789394 | 0.09464711 |
| 0.34533484 | 0.81096631 | 0.61151439 |
| 0.46564776 | 0.67609267 | 0.10835858 |
| 0.95942195 | 0.16789717 | 0.60195693 |
| 0.16496975 | 0.33052022 | 0.75853005 |
| 0.67360788 | 0.82124035 | 0.26168067 |
| 0.81574444 | 0.02739460 | 0.39892887 |
| 0.32573863 | 0.52055535 | 0.90772735 |
| 0.02012991 | 0.87705043 | 0.30898160 |
| 0.51650704 | 0.35908229 | 0.82138465 |
| 0.88017299 | 0.36979337 | 0.44638096 |
| 0.37736577 | 0.87857132 | 0.95532213 |
| 0.00846841 | 0.22764892 | 0.94019236 |
| 0.52981999 | 0.71629041 | 0.45636229 |
| 0.62962415 | 0.48681464 | 0.19450237 |
| 0.13666447 | 0.96461357 | 0.67701343 |
| 0.13219813 | 0.61722177 | 0.06309688 |
| 0.61432259 | 0.12495256 | 0.54744705 |
| 0.26293843 | 0.48445335 | 0.56192228 |
| 0.75666394 | 0.97183859 | 0.05910280 |
| 0.06356939 | 0.66705534 | 0.27144039 |
| 0.57013760 | 0.16287519 | 0.75730477 |
| 0.84178018 | 0.41225634 | 0.23904365 |
| 0.31903216 | 0.92210310 | 0.75934208 |
| 0.79626359 | 0.17741223 | 0.01684675 |
| 0.31657777 | 0.68832995 | 0.50319787 |
| 0.09564728 | 0.17995222 | 0.72493322 |
| 0.56346342 | 0.69524214 | 0.24353658 |
| 0.30954593 | 0.41912743 | 0.77231329 |
| 0.81968038 | 0.92318921 | 0.25540353 |
| 0.33710969 | 0.67184460 | 0.99325455 |
| 0.82063140 | 0.17407656 | 0.49282546 |
| 0.21963492 | 0.18518946 | 0.49529333 |
| 0.15811901 | 0.27041515 | 0.15207857 |
| 0.07925907 | 0.16542943 | 0.18947095 |
| 0.04818466 | 0.23957078 | 0.29600590 |
| 0.16817977 | 0.00433189 | 0.49226587 |
| 0.06686509 | 0.03401791 | 0.41675170 |
| 0.21218288 | 0.91101629 | 0.40022006 |
| 0.25591531 | 0.28034100 | 0.34385785 |
| 0.45433827 | 0.08021703 | 0.29614112 |
| 0.41735795 | 0.94260958 | 0.35660014 |
| 0.39446484 | 0.02243940 | 0.45631687 |
| 0.35006260 | 0.08677316 | 0.09984312 |
| 0.25238184 | 0.99530871 | 0.15590660 |

| | | |
|------------|------------|------------|
| 0.37599753 | 0.94617933 | 0.21496837 |
| 0.11130795 | 0.25424789 | 0.41165247 |
| 0.12011949 | 0.19916240 | 0.22602944 |
| 0.16440075 | 0.00381281 | 0.40578596 |
| 0.22041971 | 0.09493051 | 0.27415693 |
| 0.26766982 | 0.10946361 | 0.35166654 |
| 0.20750325 | 0.21165755 | 0.40575721 |
| 0.38888677 | 0.03217947 | 0.36842318 |
| 0.30542365 | 0.02560861 | 0.18198099 |

Type B isomerisation, configuration R7 of the reactant

| | | | | |
|---------------------------|------------|------------|----|---|
| 1 | | | | |
| -7.923688 | -0.000017 | 9.876322 | | |
| 3.961561 | -6.862259 | 9.876106 | | |
| 3.961547 | 6.862198 | 9.876070 | | |
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |
| Direct configuration= 706 | | | | |
| 0.12024029 | 0.75234497 | 0.28431320 | | |
| 0.62247900 | 0.24260542 | 0.78361512 | | |
| 0.85536209 | 0.47136215 | 0.31897263 | | |
| 0.34418035 | 0.98088100 | 0.83214647 | | |
| 0.88902063 | 0.20627345 | 0.05077264 | | |
| 0.40323496 | 0.69722469 | 0.55993830 | | |
| 0.74649910 | 0.37247423 | 0.21546326 | | |
| 0.24594277 | 0.86552650 | 0.72090995 | | |
| 0.01680089 | 0.64249040 | 0.17991897 | | |
| 0.51221707 | 0.14503284 | 0.67393782 | | |
| 0.29043093 | 0.60335205 | 0.45159574 | | |
| 0.78767328 | 0.09069409 | 0.94903049 | | |
| 0.28270605 | 0.37466165 | 0.68259034 | | |
| 0.78796021 | 0.86991425 | 0.17788928 | | |
| 0.73455972 | 0.14970701 | 0.44372204 | | |
| 0.24720614 | 0.64120143 | 0.94900250 | | |
| 0.39205148 | 0.46919247 | 0.79178290 | | |
| 0.89445591 | 0.98114753 | 0.28087952 | | |
| 0.12024406 | 0.20558672 | 0.82418109 | | |
| 0.62208996 | 0.70516767 | 0.32469677 | | |
| 0.34938636 | 0.75290613 | 0.05328810 | | |
| 0.84623727 | 0.25135089 | 0.55225204 | | |
| 0.51488434 | 0.60605514 | 0.22273153 | | |
| 0.01952777 | 0.09119634 | 0.71430408 | | |
| 0.22792223 | 0.78947324 | 0.16217679 | | |
| 0.72935211 | 0.28686124 | 0.66566244 | | |
| 0.23155736 | 0.09321290 | 0.87374086 | | |
| 0.73391799 | 0.58329021 | 0.33909474 | | |
| 0.93278824 | 0.09344799 | 0.16451597 | | |
| 0.43125051 | 0.57596950 | 0.67034899 | | |
| 0.69745559 | 0.26573849 | 0.33090928 | | |
| 0.20955312 | 0.74974483 | 0.83393811 | | |
| 0.40290503 | 0.26726665 | 0.64123408 | | |
| 0.90442139 | 0.75723962 | 0.14168497 | | |
| 0.41014326 | 0.56008158 | 0.34394004 | | |
| 0.90406562 | 0.05175004 | 0.84359988 | | |
| 0.17362533 | 0.67966347 | 0.39987067 | | |
| 0.66573339 | 0.16717359 | 0.90463041 | | |
| 0.46328521 | 0.02682075 | 0.74659969 | | |
| 0.97462118 | 0.51963920 | 0.25044550 | | |

| | | |
|------------|------------|------------|
| 0.81030245 | 0.32796005 | 0.09471772 |
| 0.34350330 | 0.81698340 | 0.60463879 |
| 0.46490690 | 0.67307040 | 0.10547669 |
| 0.96877657 | 0.17324675 | 0.58687380 |
| 0.16400847 | 0.32822267 | 0.75334213 |
| 0.66847230 | 0.82431105 | 0.26251716 |
| 0.81414803 | 0.02869756 | 0.39919345 |
| 0.32346004 | 0.51609110 | 0.91171949 |
| 0.01828515 | 0.87781283 | 0.30717799 |
| 0.51280316 | 0.36095479 | 0.81336785 |
| 0.86645281 | 0.37784924 | 0.44927973 |
| 0.37530041 | 0.87817054 | 0.95497408 |
| 0.01035474 | 0.23149392 | 0.94545185 |
| 0.53024857 | 0.71074229 | 0.45760064 |
| 0.63140105 | 0.49159503 | 0.19696773 |
| 0.13098910 | 0.96222027 | 0.68042153 |
| 0.12650149 | 0.62022078 | 0.05958430 |
| 0.61151371 | 0.12437413 | 0.54704975 |
| 0.26238415 | 0.48476715 | 0.56066403 |
| 0.75524943 | 0.97178354 | 0.05868378 |
| 0.06266506 | 0.66809042 | 0.26810591 |
| 0.57248723 | 0.15865039 | 0.75709478 |
| 0.84740478 | 0.40446846 | 0.23727215 |
| 0.31511565 | 0.92141736 | 0.76003588 |
| 0.80436271 | 0.17392071 | 0.00892190 |
| 0.31415191 | 0.69079611 | 0.49993140 |
| 0.08329080 | 0.17561613 | 0.73672641 |
| 0.55178766 | 0.70519793 | 0.24162260 |
| 0.30080323 | 0.42151231 | 0.77439108 |
| 0.81646403 | 0.92511857 | 0.25525010 |
| 0.33170706 | 0.67267164 | 0.99334964 |
| 0.81526625 | 0.17703649 | 0.49464589 |
| 0.11913755 | 0.28328818 | 0.39276703 |
| 0.07614793 | 0.13091236 | 0.19341467 |
| 0.08149201 | 0.23882258 | 0.24525934 |
| 0.18243493 | 0.21169122 | 0.09980568 |
| 0.24334362 | 0.08902488 | 0.50022492 |
| 0.10631460 | 0.07813972 | 0.43473501 |
| 0.24157037 | 0.94753295 | 0.42971526 |
| 0.25519772 | 0.29746566 | 0.38704702 |
| 0.44133198 | 0.10365506 | 0.25282399 |
| 0.44293376 | 0.97414436 | 0.38456474 |
| 0.44727388 | 0.11179920 | 0.38628640 |
| 0.37070653 | 0.90625227 | 0.24006898 |
| 0.39650247 | 0.04752343 | 0.14155848 |
| 0.31042277 | 0.99107025 | 0.11053634 |
| 0.24354411 | 0.28934828 | 0.25574183 |
| 0.13843405 | 0.17132256 | 0.19576803 |
| 0.20166662 | 0.04302553 | 0.38506135 |
| 0.22175993 | 0.06850928 | 0.25784282 |
| 0.27064390 | 0.11792259 | 0.40034589 |
| 0.21837384 | 0.25460188 | 0.35543571 |
| 0.40788103 | 0.07338537 | 0.35256733 |
| 0.32868432 | 0.99603188 | 0.18605769 |

Type B isomerisation, configuration TS7 of the TS

1.00000000000000

-7.9236880000000003 -0.0000170000000000 9.8763220000000000

3.9615610000000001 -6.8622589999999999 9.8761060000000001
3.9615469999999999 6.8621980000000002 9.8760700000000003

Si Al O H C
23 1 48 15 7

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1202653155291708 | 0.7517729158922364 | 0.2829138375580339 |
| 0.6232372839792758 | 0.2468319487241860 | 0.7804275274501301 |
| 0.8541706935550525 | 0.4724515877016513 | 0.3193910941211870 |
| 0.3482516059039810 | 0.9806142839279747 | 0.8296214276233108 |
| 0.8932503678563978 | 0.2049952065225513 | 0.0503705705965698 |
| 0.4038450085456243 | 0.6939117725528435 | 0.5574660099867569 |
| 0.7455637503326740 | 0.3717026935989481 | 0.2140742859593156 |
| 0.2484571581007292 | 0.8688327841768220 | 0.7190508848487773 |
| 0.0162602357694407 | 0.6445974595113936 | 0.1760138385691306 |
| 0.5142539488306224 | 0.1449332845578589 | 0.6733785592082373 |
| 0.2905034052094998 | 0.6017081370402179 | 0.4495529853388960 |
| 0.7944276022759447 | 0.0892579618443682 | 0.9470228713397026 |
| 0.2847347527751081 | 0.3739242833808958 | 0.6802390986415003 |
| 0.7883492425353550 | 0.8716033312841714 | 0.1763438590021077 |
| 0.7351496801025936 | 0.1494048374899733 | 0.4420310138904803 |
| 0.2431455498781738 | 0.6482983105416179 | 0.9453833811613074 |
| 0.3954701659382436 | 0.4703719195940211 | 0.7869280108533706 |
| 0.8951332837969104 | 0.9800826176982140 | 0.2809084201001169 |
| 0.1210125474764852 | 0.2077238597391726 | 0.8230740084795075 |
| 0.6233233175736307 | 0.7044371241595413 | 0.3220522897565998 |
| 0.3483050876272182 | 0.7545624752957119 | 0.0522828922908835 |
| 0.8426526476458478 | 0.2541692311018243 | 0.5513675923762845 |
| 0.5162681103636071 | 0.6046620951988622 | 0.2189685617124201 |
| 0.0197977108141249 | 0.0927525488698840 | 0.7167756771539849 |
| 0.2278573044241504 | 0.7905511371753440 | 0.1619401336521997 |
| 0.7213578225528811 | 0.2994659891976098 | 0.6566783556202294 |
| 0.2338461255841016 | 0.0933122426710617 | 0.8661284408173850 |
| 0.7315625335139313 | 0.5812111251247639 | 0.3490874944451079 |
| 0.9334038038550746 | 0.0910589359524179 | 0.1641779399260070 |
| 0.4429960629068533 | 0.5688588089085524 | 0.6600857289105544 |
| 0.6974424040408097 | 0.2640442405879141 | 0.3289301523634522 |
| 0.1978552683126495 | 0.7642845748926553 | 0.8376030699237642 |
| 0.4031012860877876 | 0.2646392992050807 | 0.6403445586239113 |
| 0.9062562867066176 | 0.7616500069155133 | 0.1361348833284386 |
| 0.4113355878211360 | 0.5617698536968621 | 0.3417844818839658 |
| 0.9158784936324833 | 0.0390419769570156 | 0.8506930086855838 |
| 0.1733373207883245 | 0.6769607958507682 | 0.3987061082457967 |
| 0.6792532158237854 | 0.1682644128015221 | 0.8925717848313834 |
| 0.4685634890611763 | 0.0250147267313106 | 0.7477744306175118 |
| 0.9711331339508205 | 0.5237675747350981 | 0.2470742333708092 |
| 0.8139452940731221 | 0.3267871081862814 | 0.0937962279977206 |
| 0.3412299680417139 | 0.8084379865192588 | 0.6101593885118725 |
| 0.4643607347912958 | 0.6728670806632975 | 0.1031301425955410 |
| 0.9581094662021616 | 0.1697700392776882 | 0.5969905262481494 |
| 0.1647239933191909 | 0.3301598275679544 | 0.7528981586762147 |
| 0.6709702667379521 | 0.8225156137498441 | 0.2591582907810372 |
| 0.8157849472247991 | 0.0275879883974248 | 0.3995374405167251 |
| 0.3221582075516900 | 0.5293534286277511 | 0.8983066949363829 |
| 0.0175155591955055 | 0.8753089351190777 | 0.3090551088612900 |
| 0.5115096997021629 | 0.3603374374034926 | 0.8199790819216582 |
| 0.8752517283050159 | 0.3746405165412625 | 0.4454780015324796 |
| 0.3751373341589829 | 0.8789148693103498 | 0.9538347371236587 |
| 0.0157126517551458 | 0.2300384806350270 | 0.9474082434879891 |

| | | |
|--------------------|--------------------|---------------------|
| 0.5238430735115390 | 0.7193871617764861 | 0.4496572706637719 |
| 0.6286257957498051 | 0.4875172486769798 | 0.1930258988454354 |
| 0.1421700264781136 | 0.9747837202376436 | 0.6669659646866695 |
| 0.1257742159062170 | 0.6189667976439952 | 0.0564737922995446 |
| 0.6130001522281103 | 0.1237899309465700 | 0.5465967034850567 |
| 0.2646911257809290 | 0.4816357908951290 | 0.5569584239277861 |
| 0.7524579362412538 | 0.9766631928819764 | 0.0598691220290118 |
| 0.0639493379680248 | 0.6681664257367123 | 0.2640463187241859 |
| 0.5731416691267591 | 0.1622999726047361 | 0.7551367332955288 |
| 0.8410125232791507 | 0.4087526998830975 | 0.2385165735169642 |
| 0.3249675129698318 | 0.9201909148320983 | 0.7534576097573209 |
| 0.8102431712121113 | 0.1760047127105934 | 0.0031095964267701 |
| 0.3104772525222650 | 0.6889451952468001 | 0.5016277773230792 |
| 0.0775844146282450 | 0.1840630227711365 | 0.7358223619669041 |
| 0.5606521899145701 | 0.6997009364989530 | 0.2352168867395364 |
| 0.3049022902966830 | 0.4223936554086387 | 0.7692390585847948 |
| 0.8156726078364657 | 0.9238334460559615 | 0.2571163712606525 |
| 0.3283121089427187 | 0.6760133637008570 | -0.0079978758242617 |
| 0.8152052608031118 | 0.1791659013217034 | 0.4918045332355869 |
| 0.0981171750770629 | 0.2638675694723610 | 0.4130697115077653 |
| 0.1269698736505283 | 0.1628503994985483 | 0.1580434770112239 |
| 0.0622483784364057 | 0.2331499845527386 | 0.2756809075777871 |
| 0.1989268625875153 | 0.2560192631577251 | 0.1603891751792740 |
| 0.2033221591991576 | 0.0473098681242358 | 0.4967163880642821 |
| 0.0687470156695077 | 0.0527275007410217 | 0.4545771419028145 |
| 0.2047263250670363 | 0.9170919811293411 | 0.4489274605804607 |
| 0.2128287618618088 | 0.2382339515114127 | 0.4735802265015950 |
| 0.4382660269482098 | 0.0922013005692646 | 0.3048378804779539 |
| 0.4191250095597875 | 0.9477367794579256 | 0.4022274520639543 |
| 0.3964156496470413 | 0.0595335276453722 | 0.4656146692380295 |
| 0.3799554740920721 | 0.9179475519837658 | 0.2656649311129833 |
| 0.3993407141068436 | 0.0576144529990991 | 0.1549113590387395 |
| 0.3040962948413243 | 0.9886253823110501 | 0.1517964669331359 |
| 0.2406706185921063 | 0.2876819526158944 | 0.3125525919215071 |
| 0.1480100211845570 | 0.1894742508004002 | 0.2179468645362125 |
| 0.1642420136469729 | 0.0137884387497803 | 0.4097167456279919 |
| 0.2230181178745257 | 0.0767199978568441 | 0.2900263312238322 |
| 0.2505310700997984 | 0.0986202740163979 | 0.3976827470529072 |
| 0.1960825711675246 | 0.2306146529384576 | 0.3987630595452535 |
| 0.3844165377270495 | 0.0450396095351532 | 0.3918913992798924 |
| 0.3336991332990156 | 0.0056052692291186 | 0.2122433116563769 |

Type B isomerisation, configuration P7 of the product

| | | |
|---------------------------|------------|------------|
| 1 | | |
| -7.923688 | -0.000017 | 9.876322 |
| 3.961561 | -6.862259 | 9.876106 |
| 3.961547 | 6.862198 | 9.876070 |
| Si | Al | O |
| 23 | 1 | 48 |
| | | 15 |
| | | 7 |
| Direct configuration= 674 | | |
| 0.11958132 | 0.75378375 | 0.28342405 |
| 0.62307628 | 0.24472643 | 0.77798602 |
| 0.85528843 | 0.47278174 | 0.32061238 |
| 0.34495105 | 0.98183956 | 0.83126487 |
| 0.88840867 | 0.20521761 | 0.05092802 |
| 0.40499759 | 0.69581385 | 0.55947606 |
| 0.74525933 | 0.37395491 | 0.21355755 |
| 0.24543344 | 0.86627730 | 0.72236269 |

| | | |
|------------|------------|------------|
| 0.01840264 | 0.64256221 | 0.17803368 |
| 0.51086307 | 0.14647594 | 0.67393477 |
| 0.29046167 | 0.60219419 | 0.45179566 |
| 0.79483662 | 0.09044726 | 0.94932914 |
| 0.28381698 | 0.37563683 | 0.68214915 |
| 0.79074706 | 0.86899708 | 0.17210478 |
| 0.73723669 | 0.14837333 | 0.44139536 |
| 0.24752081 | 0.64405717 | 0.94806773 |
| 0.39928466 | 0.47007435 | 0.78842637 |
| 0.89465660 | 0.98049097 | 0.27812211 |
| 0.12225271 | 0.20801950 | 0.82043447 |
| 0.62562970 | 0.70284969 | 0.32557533 |
| 0.34811780 | 0.75653435 | 0.05290964 |
| 0.84419412 | 0.24914595 | 0.54978102 |
| 0.51548312 | 0.60276942 | 0.22238004 |
| 0.02397807 | 0.09394144 | 0.71782997 |
| 0.22472745 | 0.79339723 | 0.15992639 |
| 0.71547880 | 0.29561370 | 0.64773274 |
| 0.23154889 | 0.09409579 | 0.87112601 |
| 0.73526877 | 0.58192680 | 0.35571861 |
| 0.93460704 | 0.09178721 | 0.16240955 |
| 0.44394195 | 0.57239295 | 0.66411140 |
| 0.69961801 | 0.26637877 | 0.33052396 |
| 0.20188572 | 0.75598943 | 0.83840499 |
| 0.40080539 | 0.26679988 | 0.63855101 |
| 0.90803998 | 0.75707020 | 0.13499527 |
| 0.41121868 | 0.55860125 | 0.34540886 |
| 0.92540173 | 0.04793764 | 0.85979271 |
| 0.17550086 | 0.68075721 | 0.39749086 |
| 0.68740655 | 0.16537594 | 0.88396828 |
| 0.46410696 | 0.02698340 | 0.74320057 |
| 0.97441786 | 0.52094276 | 0.24999642 |
| 0.81698814 | 0.32758961 | 0.09419306 |
| 0.34171793 | 0.81156664 | 0.61030656 |
| 0.46142806 | 0.67692630 | 0.10815475 |
| 0.95365736 | 0.17075929 | 0.60500767 |
| 0.16413907 | 0.33148387 | 0.76055404 |
| 0.67227718 | 0.82192533 | 0.25707434 |
| 0.80897346 | 0.02755114 | 0.39618446 |
| 0.32682393 | 0.52310729 | 0.90413694 |
| 0.01622030 | 0.87703325 | 0.30996711 |
| 0.51663936 | 0.36024727 | 0.81902284 |
| 0.87813775 | 0.36883700 | 0.44326676 |
| 0.37637541 | 0.88019449 | 0.95388950 |
| 0.00604505 | 0.22801179 | 0.93863025 |
| 0.52545985 | 0.72125402 | 0.45178882 |
| 0.62558068 | 0.48581363 | 0.19165231 |
| 0.13521309 | 0.96789721 | 0.67501482 |
| 0.13080500 | 0.61543876 | 0.06090398 |
| 0.61504396 | 0.12738422 | 0.54889352 |
| 0.25958083 | 0.48434868 | 0.56039426 |
| 0.75512490 | 0.97229644 | 0.05435465 |
| 0.06220625 | 0.66926203 | 0.26711951 |
| 0.56338293 | 0.16130477 | 0.76296243 |
| 0.83713480 | 0.41776135 | 0.23554624 |
| 0.31707418 | 0.92076973 | 0.75945858 |
| 0.79366603 | 0.17705820 | 0.01766635 |
| 0.31388654 | 0.68727763 | 0.50337552 |

| | | |
|------------|------------|------------|
| 0.09498898 | 0.18434578 | 0.72120301 |
| 0.56402721 | 0.69277828 | 0.24116918 |
| 0.30976531 | 0.42288938 | 0.76814589 |
| 0.81971129 | 0.92319454 | 0.24978971 |
| 0.33216794 | 0.67578913 | 0.99189729 |
| 0.82748701 | 0.16882843 | 0.48709189 |
| 0.10135599 | 0.26352359 | 0.40393510 |
| 0.09281296 | 0.15530437 | 0.18265948 |
| 0.05466929 | 0.24286124 | 0.27957061 |
| 0.17304067 | 0.26058068 | 0.14020028 |
| 0.16608857 | 0.00993826 | 0.49621288 |
| 0.06302022 | 0.04595908 | 0.41995441 |
| 0.20351961 | 0.91629249 | 0.40775995 |
| 0.20192857 | 0.20353674 | 0.49484696 |
| 0.44695708 | 0.09117940 | 0.31238826 |
| 0.41427857 | 0.95086134 | 0.37568289 |
| 0.37863543 | 0.03988868 | 0.47168882 |
| 0.38155697 | 0.93811977 | 0.23655956 |
| 0.36826909 | 0.07294735 | 0.11281402 |
| 0.26887992 | 0.98426569 | 0.16393211 |
| 0.24466742 | 0.29145335 | 0.34095933 |
| 0.13009007 | 0.19456442 | 0.21737532 |
| 0.16053900 | 0.01059168 | 0.40980756 |
| 0.22439353 | 0.09384373 | 0.27720956 |
| 0.26237549 | 0.11581659 | 0.35730064 |
| 0.19611533 | 0.22316503 | 0.40400587 |
| 0.38088929 | 0.04296968 | 0.38291360 |
| 0.31679332 | 0.01682459 | 0.19393678 |

Type A isomerisation, configuration R1 of the reactant

1.000000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1206784065696901 | 0.7374313755290658 | 0.2768092727197067 |
| 0.6209189797487401 | 0.2318987458660589 | 0.7792193188893110 |
| 0.8517403251440923 | 0.4626953967889229 | 0.3118939293044378 |
| 0.3460985206079412 | 0.9660669369913625 | 0.8242925866643848 |
| 0.8907991035458364 | 0.1921115760253493 | 0.0452124617429654 |
| 0.4010999894205032 | 0.6851025347875803 | 0.5529449143751881 |
| 0.7453620344836065 | 0.3588438049621249 | 0.2099841257687325 |
| 0.2460251118333059 | 0.8562176323871296 | 0.7101813696392203 |
| 0.0150295903020013 | 0.6313526136689613 | 0.1726712494186956 |
| 0.5144923892371078 | 0.1310149637959247 | 0.6684023452308407 |
| 0.2893616538646874 | 0.5876960393076121 | 0.4454157201961197 |
| 0.7864751897999573 | 0.0811652002952858 | 0.9415356795930595 |
| 0.2838708468172569 | 0.3617994274562855 | 0.6727867636805019 |
| 0.7826398822496025 | 0.8621216738064352 | 0.1753099101065347 |
| 0.7356873865000699 | 0.1369825907204536 | 0.4395517762412636 |
| 0.2417490202566829 | 0.6314118860524729 | 0.9403100840455635 |
| 0.3908017203978945 | 0.4607554789682886 | 0.7824281002246237 |
| 0.8916921069154943 | 0.9681581476573596 | 0.2765680828563948 |
| 0.1206135449610475 | 0.1919532938600988 | 0.8198049555406022 |
| 0.6186940381968126 | 0.6965769008919225 | 0.3130712778701096 |
| 0.3467989269749833 | 0.7390568376227650 | 0.0468111685743633 |

| | | |
|--------------------|--------------------|--------------------|
| 0.8427602115718379 | 0.2448685535576909 | 0.5475360736009933 |
| 0.5143720264194944 | 0.5925917910560298 | 0.2137621989756944 |
| 0.0173457533510997 | 0.0817768110049442 | 0.7073779260171288 |
| 0.2268597156279131 | 0.7783476729040116 | 0.1554029809960106 |
| 0.7291129025605353 | 0.2780092937283928 | 0.6641037522027163 |
| 0.2322042895271404 | 0.0776788726402255 | 0.8648186135664803 |
| 0.7335094564134663 | 0.5777110815213604 | 0.3288258473921606 |
| 0.9312717287106433 | 0.0768707780384853 | 0.1576377851718560 |
| 0.4357933699825814 | 0.5678164534424883 | 0.6651372337684113 |
| 0.6971672963984296 | 0.2519817107737871 | 0.3265400037369611 |
| 0.2089667749738685 | 0.7409880577439368 | 0.8238821304179110 |
| 0.4050199899920533 | 0.2532526119757365 | 0.6353929612282331 |
| 0.9012979473737842 | 0.7487307304009324 | 0.1443502391971734 |
| 0.4108671587353872 | 0.5483388212908780 | 0.3375319237623395 |
| 0.8987002560832638 | 0.0434364796378260 | 0.8322017240805583 |
| 0.1734566442129613 | 0.6655810531761649 | 0.3928019034217686 |
| 0.6614922489243737 | 0.1577148476244504 | 0.9019430881547065 |
| 0.4650874713457567 | 0.0133721738711644 | 0.7415989815917622 |
| 0.9732327121267972 | 0.5079636725259747 | 0.2432694321910361 |
| 0.8110434877742645 | 0.3130457212618212 | 0.0902936852091509 |
| 0.3410925734415463 | 0.8073521953892848 | 0.5935973444862868 |
| 0.4623791074385596 | 0.6550980113421706 | 0.0981845068213769 |
| 0.9690406822612875 | 0.1716048642603804 | 0.5779069895613292 |
| 0.1664934295080902 | 0.3134649173944068 | 0.7467413205870105 |
| 0.6617108868033714 | 0.8176912654680745 | 0.2528503790292243 |
| 0.8195203039425274 | 0.0168536880940784 | 0.3950904811945010 |
| 0.3179439312011656 | 0.5055547504070080 | 0.9038053559454191 |
| 0.0117538764888851 | 0.8577092891926620 | 0.3013918488011028 |
| 0.5077910396390323 | 0.3484784821617041 | 0.8085406434765092 |
| 0.8595241887504426 | 0.3720809244322515 | 0.4443181341290311 |
| 0.3768016068153585 | 0.8606997180608140 | 0.9451449801597896 |
| 0.0124520837129502 | 0.2183002231904153 | 0.9409717483248904 |
| 0.5248046839529079 | 0.6990598267355970 | 0.4455292157475269 |
| 0.6283150440472638 | 0.4752519572386356 | 0.1902061320756382 |
| 0.1307732765152648 | 0.9552795144723857 | 0.6722592385590347 |
| 0.1177822313027619 | 0.6128488687014390 | 0.0471759683059532 |
| 0.6114433528256581 | 0.1098610534829913 | 0.5403019875823388 |
| 0.2617697066974560 | 0.4643582988687741 | 0.5471232210777616 |
| 0.7581248864917891 | 0.9615742225086130 | 0.0518653733695187 |
| 0.0723010904565593 | 0.6460987032155907 | 0.2587067659731496 |
| 0.5769798452420233 | 0.1463185016181744 | 0.7481654683960837 |
| 0.8428694864965669 | 0.3948249770489401 | 0.2322399603802758 |
| 0.3194451161044001 | 0.9100141963727288 | 0.7468791006634969 |
| 0.8067106778670761 | 0.1651485169842798 | 0.9973633796232646 |
| 0.3097067048029441 | 0.6677628858611717 | 0.5043220899408898 |
| 0.0798497817723866 | 0.1667261052887044 | 0.7313330417403540 |
| 0.5549901157514775 | 0.6920006926200511 | 0.2269684404767351 |
| 0.3007742814476805 | 0.4188639070324135 | 0.7564510932981698 |
| 0.8025340487556033 | 0.9192791448405434 | 0.2572072897824997 |
| 0.3244473249812473 | 0.6584019981310563 | 0.9905591300044516 |
| 0.8095215504772018 | 0.1681811699803791 | 0.4950295709658408 |
| 0.1709802243492397 | 0.3418608612117750 | 0.2073920197848901 |
| 0.4306902921660235 | 0.3602059833511764 | 0.2699807134342830 |
| 0.4200670273698689 | 0.3866699533035221 | 0.1239772800724840 |
| 0.2892508130263934 | 0.4446253656594823 | 0.2358179127250419 |
| 0.1461295667248634 | 0.3210146806699968 | 0.5208968999850534 |
| 0.1227616911582391 | 0.3866722137016505 | 0.3696378701992002 |
| 0.0944888915204639 | 0.2458906086326643 | 0.4756813300009994 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3032969728085698 | 0.2909586752717945 | 0.0944212115190975 |
| 0.4412112381800392 | 0.0593439220470668 | 0.2610187198355564 |
| 0.5242112237573745 | 0.1371620794110679 | 0.2720386877368262 |
| 0.4989765994230818 | 0.1709633501752221 | 0.1319153710118730 |
| 0.4245486009640347 | 0.1421495789021023 | 0.4652336668757335 |
| 0.3615890878769031 | 0.0433503850949847 | 0.4651293516570376 |
| 0.2802167921834680 | 0.1267848150866085 | 0.5760382221316406 |
| 0.2309260318471009 | 0.1841311635634301 | 0.2173673047742978 |
| 0.3715665185559322 | 0.3685779262181287 | 0.2214847871974036 |
| 0.1575173839273584 | 0.3049839152283310 | 0.4370148849374752 |
| 0.2768186255936617 | 0.2285427348046567 | 0.3932665499476101 |
| 0.3400962698638171 | 0.2475438664042824 | 0.2614859222345445 |
| 0.2546465534207928 | 0.2675710449309131 | 0.1917484174027048 |
| 0.4578516787435603 | 0.1474971311720451 | 0.2307786970588997 |
| 0.3360190560839527 | 0.1309779428664810 | 0.4822339619734375 |

Type A isomerization, configuration TS1 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

Si Al O H C

23 1 48 15 7

direct

| | | |
|----------------|----------------|----------------|
| 0.111409211688 | 0.739493933429 | 0.278934384797 |
| 0.618823852375 | 0.237135204743 | 0.771483018080 |
| 0.847247943285 | 0.464644492006 | 0.314256326723 |
| 0.338958440006 | 0.970839992990 | 0.826839138613 |
| 0.882549359536 | 0.194028043529 | 0.045640923823 |
| 0.396639652769 | 0.687616781112 | 0.553027139753 |
| 0.734444728551 | 0.362577809340 | 0.208517685753 |
| 0.241976754277 | 0.857065588571 | 0.714333562085 |
| 0.011914095192 | 0.631204263710 | 0.171934247803 |
| 0.504780967693 | 0.135827117347 | 0.667189640977 |
| 0.281926926050 | 0.593067245704 | 0.448523568819 |
| 0.787351715553 | 0.082363188474 | 0.941620121678 |
| 0.276668770958 | 0.365371639528 | 0.676098607023 |
| 0.782840537122 | 0.860368287180 | 0.167571670400 |
| 0.727570512762 | 0.137669690839 | 0.437058666581 |
| 0.242484693312 | 0.633898588975 | 0.940639707585 |
| 0.393033812717 | 0.461952561991 | 0.780870749986 |
| 0.886406298352 | 0.969280053447 | 0.274192107546 |
| 0.114894914531 | 0.198271222222 | 0.814241922090 |
| 0.621015243508 | 0.692706136100 | 0.316812155462 |
| 0.339948501419 | 0.745316243335 | 0.048036205313 |
| 0.839153400193 | 0.241384591172 | 0.543583911242 |
| 0.509891802497 | 0.590937046452 | 0.216045823427 |
| 0.019190006656 | 0.085228349320 | 0.706703234229 |
| 0.215062645785 | 0.778977197765 | 0.154242074819 |
| 0.717226847142 | 0.288713994020 | 0.648318200290 |
| 0.224832573504 | 0.084154541430 | 0.862816062983 |
| 0.733715453159 | 0.577725993965 | 0.351414193167 |
| 0.926313723552 | 0.079557066869 | 0.157216529112 |
| 0.437978832803 | 0.565650942791 | 0.658896547268 |
| 0.689805911707 | 0.252666719450 | 0.323447033899 |
| 0.200682862972 | 0.744261122670 | 0.829016492689 |
| 0.392485846522 | 0.254805059713 | 0.632873584598 |
| 0.901649366682 | 0.748563996027 | 0.133121896159 |

| | | |
|----------------|----------------|----------------|
| 0.405874353660 | 0.553105510545 | 0.342548756973 |
| 0.914653563353 | 0.044873478670 | 0.846714608342 |
| 0.168525205768 | 0.667855416370 | 0.392134434230 |
| 0.673452447400 | 0.155502987811 | 0.884559318837 |
| 0.459081693790 | 0.016214676438 | 0.743256785018 |
| 0.968659755971 | 0.509064569308 | 0.236658515542 |
| 0.811074385140 | 0.316394094611 | 0.089370887943 |
| 0.339613999288 | 0.804694574783 | 0.600858025026 |
| 0.452541739278 | 0.666547090313 | 0.104508924695 |
| 0.953425647239 | 0.160358303185 | 0.590483357156 |
| 0.156925826519 | 0.321904879807 | 0.755772307366 |
| 0.662646766552 | 0.815010955982 | 0.248171036078 |
| 0.804860371985 | 0.016756568127 | 0.392807265197 |
| 0.319472497935 | 0.510960110571 | 0.899323608087 |
| 0.005942959053 | 0.861532420870 | 0.304393754497 |
| 0.509602183803 | 0.351404965722 | 0.812357732663 |
| 0.871084106530 | 0.360906954840 | 0.435847675907 |
| 0.367224800285 | 0.869755858657 | 0.950819946910 |
| 0.999900702398 | 0.216971001739 | 0.933490164099 |
| 0.514836855210 | 0.708619438550 | 0.440003348383 |
| 0.610211450654 | 0.467810489926 | 0.186473823586 |
| 0.129868532067 | 0.957132632155 | 0.671965537322 |
| 0.124391189369 | 0.608438428376 | 0.053288622633 |
| 0.602478121369 | 0.114743932546 | 0.539378164093 |
| 0.254273337194 | 0.470267187615 | 0.551470187608 |
| 0.752269808253 | 0.962424003859 | 0.047184905642 |
| 0.057174349916 | 0.650212887988 | 0.265166886040 |
| 0.563883199001 | 0.156540621607 | 0.746168259454 |
| 0.817667761388 | 0.413547733290 | 0.233733760706 |
| 0.315149097019 | 0.908753881546 | 0.753258869662 |
| 0.787112618840 | 0.168850928138 | 0.010017318717 |
| 0.299920508965 | 0.674541963179 | 0.507578544968 |
| 0.086390786413 | 0.177711681682 | 0.713894436095 |
| 0.572514747196 | 0.673064112008 | 0.227460027453 |
| 0.304967994410 | 0.414996488690 | 0.757973717570 |
| 0.804898181030 | 0.916701809141 | 0.248493235466 |
| 0.328730034620 | 0.662615161320 | 0.985439886362 |
| 0.806497305078 | 0.166309193061 | 0.488213790340 |
| 0.283226274115 | 0.364271165100 | 0.155818416717 |
| 0.368079631137 | 0.305880971218 | 0.436913639574 |
| 0.480340519092 | 0.314493341973 | 0.297321723538 |
| 0.325114592422 | 0.408138281240 | 0.300181249525 |
| 0.144280072561 | 0.292606336551 | 0.477853693073 |
| 0.159264141590 | 0.342740307960 | 0.319028334531 |
| 0.144021486576 | 0.195577305642 | 0.411345131808 |
| 0.442287444115 | 0.341374429696 | 0.078654914319 |
| 0.526322478187 | 0.055875817167 | 0.215058419843 |
| 0.562483349608 | 0.086956484150 | 0.318193061686 |
| 0.595324245705 | 0.172356721226 | 0.160836808472 |
| 0.442306822896 | 0.080928321411 | 0.484578031222 |
| 0.341494232976 | 0.020900442661 | 0.477606203870 |
| 0.284571191194 | 0.121519108340 | 0.565995780288 |
| 0.372051454458 | 0.236925337109 | 0.099353111341 |
| 0.383471065387 | 0.321396264184 | 0.340325081458 |
| 0.184743802034 | 0.265097437758 | 0.394446754902 |
| 0.319334915302 | 0.206605199029 | 0.374420262364 |
| 0.404991710209 | 0.216454271317 | 0.257483170318 |
| 0.372245659835 | 0.296583061619 | 0.142754936265 |

0.529952125407 0.129178060285 0.238152189387
0.350211354534 0.101964111913 0.481817341650

Type A isomerisation, configuration P1 of the product

1.000000000000000000

-7.9236879999800003 -0.0000170000000000 9.8763219999890008
3.9615609999979999 -6.8622589999810000 9.8761060000119993
3.9615470000010000 6.8621979999780001 9.8760699999810004

Si Al O H C
23 1 48 15 7

Direct

0.1152942634926993 0.7434661599463622 0.2789318859244251
0.6175533585411105 0.2324107957175711 0.7765362416518281
0.8504522096532812 0.4632078756926224 0.3137606735895442
0.3377943654579401 0.9720155747392076 0.8260419686946805
0.8821736457743339 0.1972367822785050 0.0448426800510185
0.4008905241342884 0.6860320493400851 0.5565635561948856
0.7408418913661950 0.3647767916600647 0.2084021403402477
0.2402993414478423 0.8556318389171325 0.7157260668437636
0.0136848820982072 0.6317563979985349 0.1764039442299683
0.5066239496040660 0.1364445643607657 0.6664440797977802
0.2862748424650435 0.5929238427274779 0.4467400165529634
0.7840367025352138 0.0825512914642861 0.9438193172418492
0.2762472106738673 0.3680106224191212 0.6763908723095736
0.7846125753376846 0.8608073649884898 0.1719449767294184
0.7269403562134926 0.1428066653136469 0.4368237547234642
0.2433408321438790 0.6318308252907467 0.9438946736789771
0.3881010297585735 0.4609545605256472 0.7858953493365247
0.8894125606866866 0.9734755352914388 0.2742152346710769
0.1147600243661488 0.1974494610986151 0.8147757543594496
0.6178283290727866 0.6973243538874214 0.3186370583111966
0.3433885996868211 0.7456730221750327 0.0472240024082228
0.8379327031100777 0.2446712175808229 0.5474548605721881
0.5100293832654997 0.5975860863290474 0.2167360302369542
0.0170144672720194 0.0840722600398823 0.7059456772012631
0.2200189122872004 0.7811747800156190 0.1543887693726264
0.7208789195920289 0.2838170119443721 0.6600650644546577
0.2236782143160581 0.0838140305144878 0.8660399126387568
0.7320623864744911 0.5780872150762131 0.3335134726800408
0.9274201334928792 0.0839843481330150 0.1563625603537690
0.4349989782896471 0.5661516151669215 0.6673515371207420
0.6899688440173349 0.2578063766790823 0.3227792902097489
0.2046654597935005 0.7391473747264526 0.8292020548041019
0.3977216078529976 0.2604737515647305 0.6371711209780444
0.9015693077699179 0.7476842600234576 0.1388487492197063
0.4068230629636006 0.5500693376441995 0.3391981115187104
0.9053219868334325 0.0484735714826900 0.8415556566012867
0.1713947117363860 0.6730081679748482 0.3927765275316557
0.6632104123029569 0.1550998844946231 0.8964983297783495
0.4561070798925910 0.0196120219303748 0.7393962245045750
0.9712713869265953 0.5091484352544352 0.2443892328848267
0.8072369221723776 0.3198570801056697 0.0878952119092565
0.3385771475829085 0.8060390429282451 0.6005815921571165
0.4576006987344260 0.6657053908903985 0.1013744014769587
0.9582790842389490 0.1640422445349489 0.5843548718928510
0.1587926161258536 0.3200620498371815 0.7511941016463212
0.6626690089782122 0.8181825211823529 0.2550241449075547
0.8085199483077237 0.0223320883894462 0.3920588853903666

| | | |
|--------------------|--------------------|--------------------|
| 0.3197514732663000 | 0.5053630157597664 | 0.9078854029043373 |
| 0.0100697746474738 | 0.8665612089550606 | 0.3026842538263835 |
| 0.5027949705206585 | 0.3452898228907275 | 0.8130846637756458 |
| 0.8603463918100870 | 0.3701480232238582 | 0.4443228578884222 |
| 0.3705600445697305 | 0.8694769129814720 | 0.9477653464599364 |
| 0.9992773510248907 | 0.2210991952876152 | 0.9326806222037529 |
| 0.5255797745317911 | 0.7026824578314226 | 0.4512414573261608 |
| 0.6244199289874849 | 0.4820832666574033 | 0.1884098337687749 |
| 0.1245846222505388 | 0.9519766875014397 | 0.6773773743970705 |
| 0.1238060277888811 | 0.6095919831131157 | 0.0560616574314144 |
| 0.6014803540660301 | 0.1172754664865604 | 0.5366150261080103 |
| 0.2546960884850923 | 0.4726674590123485 | 0.5514071916500051 |
| 0.7536995416409644 | 0.9612792533401054 | 0.0509744523472401 |
| 0.0602023560274927 | 0.6543596054611525 | 0.2660750114088055 |
| 0.5729973859010355 | 0.1470140100602412 | 0.7460009276753854 |
| 0.8381945140319715 | 0.3984957181828768 | 0.2330348251212953 |
| 0.3107404796448739 | 0.9108832125499375 | 0.7540269737836407 |
| 0.7884904814326820 | 0.1680470504180614 | 0.0102943722668532 |
| 0.3117447391713686 | 0.6718921586216084 | 0.5026925321881376 |
| 0.0845234439639350 | 0.1724453809338806 | 0.7186884590606369 |
| 0.5505991631593247 | 0.6939237650410395 | 0.2351060696866694 |
| 0.2941497182607922 | 0.4228549864752180 | 0.7616472962121511 |
| 0.8077856391788150 | 0.9193947756551129 | 0.2501066647350744 |
| 0.3288836453614364 | 0.6624654763896058 | 0.9875864536057960 |
| 0.8010475161077919 | 0.1730602388702455 | 0.4920672587769541 |
| 0.3466732134845656 | 0.3226539788106643 | 0.1008557260613442 |
| 0.2581601451966918 | 0.3649699274769318 | 0.4162076396820125 |
| 0.4192266316527086 | 0.3190266125614795 | 0.3531024011954495 |
| 0.3232122676218757 | 0.4064574679591262 | 0.2548524353401470 |
| 0.1192028187371081 | 0.2693495543696313 | 0.4170463719091947 |
| 0.1730018789380036 | 0.3204698630648952 | 0.2560693400957482 |
| 0.1776046967171550 | 0.1647564939878595 | 0.3331999692045256 |
| 0.4832080313545229 | 0.2080007976857205 | 0.0524652248850597 |
| 0.5512586065677761 | 0.0276727959934141 | 0.2614901473516969 |
| 0.5520061688271085 | 0.1178795908899025 | 0.3372888061591133 |
| 0.6089847805009171 | 0.1521895883182315 | 0.1719601096160981 |
| 0.4096941842532918 | 0.1096238178053688 | 0.4894976233319893 |
| 0.3257058848319420 | 0.0337114415439005 | 0.4768620441061335 |
| 0.2486397211434287 | 0.1549254890764654 | 0.5434902990181699 |
| 0.3369330548737125 | 0.1792269199920759 | 0.1336197609275078 |
| 0.3326075755110571 | 0.3353826160476033 | 0.3402449343890716 |
| 0.1891252013714665 | 0.2446915812391604 | 0.3367544639104161 |
| 0.3144548253074359 | 0.2144651852604533 | 0.3489255160315879 |
| 0.4166529823495115 | 0.1875166908417165 | 0.2442448703275630 |
| 0.3987582671901565 | 0.2256808894674716 | 0.1251046733762361 |
| 0.5390319535769899 | 0.1225509257980997 | 0.2549758442059407 |
| 0.3268244765372184 | 0.1220761389117428 | 0.4717574708307735 |

Type A isomerisation, configuration R2 of the reactant

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1142677847248096 | 0.7537864789547613 | 0.2766420532418219 |
| 0.6178509497518554 | 0.2418123300350171 | 0.7743904591196089 |

| | | |
|--------------------|--------------------|--------------------|
| 0.8467957389410646 | 0.4734708436912221 | 0.3134303765181082 |
| 0.3379538674655629 | 0.9828922345996415 | 0.8230808245789033 |
| 0.8822387334951167 | 0.2064073014558140 | 0.0424557792355779 |
| 0.4013299449886988 | 0.6926335581275347 | 0.5532303735930014 |
| 0.7398745493943970 | 0.3747808565591379 | 0.2050112350804251 |
| 0.2381149952922547 | 0.8654213903195036 | 0.7167748412657915 |
| 0.0131234837012317 | 0.6419317113900074 | 0.1729102473923011 |
| 0.5066362570129078 | 0.1470970314202065 | 0.6644111107953768 |
| 0.2848897699953155 | 0.6029955437651132 | 0.4435578635488160 |
| 0.7854831059675411 | 0.0920593606132534 | 0.9407556802342462 |
| 0.2751510988666294 | 0.3786818963219732 | 0.6756786302436781 |
| 0.7847190259451802 | 0.8713277766604480 | 0.1675383116265004 |
| 0.7259272541688062 | 0.1525898874734459 | 0.4339111241910500 |
| 0.2396894384514436 | 0.6444098419371415 | 0.9426787810764489 |
| 0.3897146337603190 | 0.4701305342787120 | 0.7807279083856018 |
| 0.8872767613672461 | 0.9833231836148932 | 0.2718846156106391 |
| 0.1147196749155322 | 0.2077598272210546 | 0.8114556759934004 |
| 0.6165146643218028 | 0.7066210648522588 | 0.3164997190891913 |
| 0.3415675513364513 | 0.7571213663512154 | 0.0460705775735737 |
| 0.8373640919985926 | 0.2532136375575488 | 0.5448908767946596 |
| 0.5085771652994281 | 0.6060743480040934 | 0.2139460812871938 |
| 0.0176815332878378 | 0.0950809918124813 | 0.7025995562462400 |
| 0.2199378002283370 | 0.7941978873665645 | 0.1541529003242045 |
| 0.7202660190021197 | 0.2940428916389683 | 0.6563866631786511 |
| 0.2238509618582356 | 0.0943000869733601 | 0.8627636665645623 |
| 0.7250755205937089 | 0.5838043882708203 | 0.3409744782020313 |
| 0.9271532144013461 | 0.0934626341284764 | 0.1546803737863282 |
| 0.4423594046456925 | 0.5666303052053387 | 0.6545287951504875 |
| 0.6904601829442684 | 0.2673213882736084 | 0.3195174419928502 |
| 0.1915033006706226 | 0.7596154865037487 | 0.8363679885291384 |
| 0.3971646764437304 | 0.2710980853844246 | 0.6379685486150146 |
| 0.9043412085426898 | 0.7604052394979152 | 0.1330028964587439 |
| 0.4040013420147204 | 0.5594637104334488 | 0.3354133256490148 |
| 0.9087064115005172 | 0.0569884446831924 | 0.8393291827048356 |
| 0.1686288008713756 | 0.6826476678081681 | 0.3917625332171397 |
| 0.6664605244070824 | 0.1644414876997322 | 0.8916109576253718 |
| 0.4563961399159698 | 0.0297423091963493 | 0.7356476948910643 |
| 0.9646440828307062 | 0.5234230339435189 | 0.2439658664724219 |
| 0.8088835024666512 | 0.3296070555921186 | 0.0847314389909226 |
| 0.3371367998127066 | 0.8045218595230085 | 0.6097822521200895 |
| 0.4570895977002293 | 0.6769531832046116 | 0.0979654126399292 |
| 0.9581903871619434 | 0.1718223754374557 | 0.5814816450887688 |
| 0.1575349966608703 | 0.3309058112334435 | 0.7486177234782435 |
| 0.6655678097956490 | 0.8242476593475446 | 0.2498605502543317 |
| 0.8064031612297118 | 0.0312955716365493 | 0.3903587568494304 |
| 0.3224077971519687 | 0.5265383331816033 | 0.8941988689545679 |
| 0.0074055171463406 | 0.8756170973537917 | 0.3012637627294464 |
| 0.5021242121156186 | 0.3537929917468428 | 0.8117535384605330 |
| 0.8623026470928227 | 0.3771501925642171 | 0.4409991820100138 |
| 0.3696179024479612 | 0.8798294053711381 | 0.9445978539502008 |
| 0.9994972838704455 | 0.2295766541085060 | 0.9297146003442579 |
| 0.5203547351105813 | 0.7234683843738503 | 0.4455436096578959 |
| 0.6224969153221912 | 0.4908733157582267 | 0.1846836569560500 |
| 0.1303604330344220 | 0.9664234682028512 | 0.6651483295566574 |
| 0.1234786230496346 | 0.6128480104131959 | 0.0547527316911523 |
| 0.5997291617115099 | 0.1290307034495748 | 0.5337034602354649 |
| 0.2549568921644826 | 0.4839841699020201 | 0.5508574765503169 |
| 0.7546309571373543 | 0.9703877863619368 | 0.0461855495889957 |

| | | |
|--------------------|--------------------|--------------------|
| 0.0627650473233222 | 0.6639487867476450 | 0.2605061963488242 |
| 0.5743701879667740 | 0.1554647067329093 | 0.7437480956202739 |
| 0.8347625561056604 | 0.4116097082480222 | 0.2301736031250817 |
| 0.3122396984258527 | 0.9229083758213632 | 0.7481290051840134 |
| 0.7895534153512824 | 0.1768512145881499 | 0.0077139737077629 |
| 0.3113180875085881 | 0.6853974266334203 | 0.4954762198963538 |
| 0.0875161694250916 | 0.1821716168446892 | 0.7135300906899191 |
| 0.5493169234690016 | 0.7009916947036220 | 0.2345255079210228 |
| 0.2911751899791334 | 0.4329056076875489 | 0.7627009089157751 |
| 0.8052961997132783 | 0.9299571250207157 | 0.2475390948354707 |
| 0.3236285146438628 | 0.6745792073559221 | 0.9885511228220366 |
| 0.8010215855037830 | 0.1810858212903100 | 0.4896861658364783 |
| 0.3045491861299108 | 0.3824268316733309 | 0.3651918431406873 |
| 0.5021741329109350 | 0.2129392620102712 | 0.2174783324341740 |
| 0.4109646239258910 | 0.1970613737898128 | 0.1505840206107645 |
| 0.3856096434061363 | 0.3411299673981711 | 0.1636038608833395 |
| 0.5004064219023781 | 0.9368306324357386 | 0.4135237638426461 |
| 0.5104915799411506 | 0.0791060468934914 | 0.4077170155784954 |
| 0.4094021918470263 | 0.0036972271137364 | 0.5313218257943326 |
| 0.2545159407468933 | 0.2713050749973597 | 0.5011448665820935 |
| 0.1143432763691631 | 0.2587172006632201 | 0.4004346503538483 |
| 0.1795145362980771 | 0.2575291984134626 | 0.2453819837176114 |
| 0.1671127117188808 | 0.3812740351926598 | 0.2853625025848282 |
| 0.2281868927796016 | 0.0696231629851154 | 0.3149474383474761 |
| 0.2132129484837820 | 0.0119298185006401 | 0.4722267226115214 |
| 0.3360508247272898 | 0.9288508399782679 | 0.3758713086911581 |
| 0.4130286101466771 | 0.2514840472433360 | 0.4240669621746679 |
| 0.4110824790679312 | 0.2427119561499483 | 0.2079520847222628 |
| 0.4507220174023140 | 0.0252388569422128 | 0.4310709359755052 |
| 0.3481554822641558 | 0.0907247150175832 | 0.3805842452524659 |
| 0.3112001549119103 | 0.2241550407420046 | 0.3354303015427216 |
| 0.3227604815825638 | 0.2847360540898656 | 0.4118116265987383 |
| 0.1855401234722594 | 0.2824581938154386 | 0.3158661512916930 |
| 0.2818566859528711 | 0.0214452121233134 | 0.3792665044955029 |

Type A isomerization, configuration TS2 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

Si Al O H C

23 1 48 15 7

direct

| | | |
|----------------|----------------|----------------|
| 0.114627553012 | 0.754209035348 | 0.277169202093 |
| 0.615654849155 | 0.242797537239 | 0.777054183812 |
| 0.848006622008 | 0.473749864054 | 0.314942350732 |
| 0.337822710671 | 0.981578452474 | 0.822457161622 |
| 0.880972158496 | 0.207571664446 | 0.044121720108 |
| 0.399169397235 | 0.696450097092 | 0.554368816501 |
| 0.740783511148 | 0.374965743353 | 0.207046361885 |
| 0.238157862209 | 0.866492667321 | 0.714337807061 |
| 0.011956268763 | 0.643624479793 | 0.174222929162 |
| 0.506172447998 | 0.146944553865 | 0.666326970642 |
| 0.285578037526 | 0.600955287099 | 0.443939947195 |
| 0.780079315653 | 0.096332578135 | 0.944470059558 |
| 0.274856772731 | 0.378712746908 | 0.675312908159 |
| 0.782408570686 | 0.872596050519 | 0.170895814010 |
| 0.725852138770 | 0.153959561570 | 0.434925354723 |

| | | |
|----------------|----------------|----------------|
| 0.241230419404 | 0.641898009571 | 0.943466743722 |
| 0.386247279267 | 0.472696335221 | 0.783999605821 |
| 0.886856396597 | 0.983710828013 | 0.273946458129 |
| 0.113796313815 | 0.207500646823 | 0.812524034741 |
| 0.615632266750 | 0.706903603426 | 0.318672846074 |
| 0.342205782814 | 0.755973802463 | 0.046271743546 |
| 0.836609114034 | 0.255219945766 | 0.546798637948 |
| 0.508589829144 | 0.606599268990 | 0.215162354360 |
| 0.014188715482 | 0.096537602665 | 0.705530588114 |
| 0.220154292576 | 0.793407720586 | 0.153992046200 |
| 0.720822411995 | 0.292145720966 | 0.660814513014 |
| 0.222492334403 | 0.092318849596 | 0.862557397543 |
| 0.727794305920 | 0.586454579257 | 0.336528588892 |
| 0.925568340348 | 0.093598894703 | 0.155774696351 |
| 0.433456340376 | 0.578476499593 | 0.665897478296 |
| 0.689215568698 | 0.267469495046 | 0.319860550171 |
| 0.203689694018 | 0.750691836382 | 0.828743753796 |
| 0.396939347356 | 0.270888623914 | 0.637799554227 |
| 0.900947808728 | 0.760841479513 | 0.137023411464 |
| 0.404419737248 | 0.557405681659 | 0.335410947177 |
| 0.901283225178 | 0.064331775773 | 0.840662592031 |
| 0.169735128189 | 0.683232596648 | 0.391755889524 |
| 0.658877504924 | 0.167464505732 | 0.898189371109 |
| 0.455915027793 | 0.029840615238 | 0.737433438528 |
| 0.967114855332 | 0.522415349705 | 0.244465167392 |
| 0.810458013175 | 0.331059335165 | 0.086028469995 |
| 0.332009382188 | 0.817552370831 | 0.597239850587 |
| 0.457764216591 | 0.677026145407 | 0.098660074882 |
| 0.958071934031 | 0.172857714503 | 0.581720088124 |
| 0.158093825809 | 0.329772805536 | 0.751538619580 |
| 0.662435574497 | 0.826359570272 | 0.251772722991 |
| 0.808010723306 | 0.032364652575 | 0.392196778650 |
| 0.318352905398 | 0.516735223487 | 0.905875417380 |
| 0.007810067619 | 0.876231022579 | 0.301405168881 |
| 0.501106388429 | 0.357229787345 | 0.809223616843 |
| 0.860217322657 | 0.381078426944 | 0.445084254520 |
| 0.369436235422 | 0.878719510399 | 0.944377245359 |
| 0.998621428152 | 0.228611483533 | 0.931144823949 |
| 0.523484571096 | 0.717195273792 | 0.450376406265 |
| 0.624777087837 | 0.492678741722 | 0.186106729186 |
| 0.121824836920 | 0.963895160926 | 0.678186407551 |
| 0.120319413404 | 0.619714364215 | 0.053506811440 |
| 0.600918015869 | 0.129142783569 | 0.536179975054 |
| 0.253420531488 | 0.481558621903 | 0.549453061342 |
| 0.751942752462 | 0.973402009093 | 0.050202282659 |
| 0.061851410353 | 0.664448850897 | 0.262345419264 |
| 0.572328938271 | 0.156164518118 | 0.746739133786 |
| 0.836665872943 | 0.408082205881 | 0.234701077489 |
| 0.313893976224 | 0.920933161300 | 0.747214578576 |
| 0.784804472052 | 0.180957235502 | 0.011233968231 |
| 0.314063561579 | 0.679645425312 | 0.497928892754 |
| 0.084183974554 | 0.185537460520 | 0.713837744296 |
| 0.546307788931 | 0.702483348119 | 0.237774133893 |
| 0.291596098765 | 0.436674571477 | 0.758569186402 |
| 0.803285048422 | 0.929987411653 | 0.251894600084 |
| 0.325042679389 | 0.671842861306 | 0.989852410697 |
| 0.799756540929 | 0.186427834054 | 0.488582117489 |
| 0.243192974819 | 0.380248527647 | 0.383378663474 |

| | | |
|----------------|----------------|----------------|
| 0.475603494921 | 0.257455873954 | 0.239712592818 |
| 0.473797175579 | 0.167491474606 | 0.160231799773 |
| 0.360702193921 | 0.307042174697 | 0.163377541572 |
| 0.555538044934 | 0.990209568933 | 0.357243120880 |
| 0.489229337896 | 0.106300116296 | 0.431512373005 |
| 0.436514105656 | 0.976389393159 | 0.494238485849 |
| 0.210235668016 | 0.257791913730 | 0.513268346894 |
| 0.106579960081 | 0.214337701647 | 0.398365284807 |
| 0.185103409239 | 0.214871827668 | 0.244094219409 |
| 0.137656026005 | 0.348768685509 | 0.287442358149 |
| 0.309006812834 | 0.056924805701 | 0.235753479373 |
| 0.314986492261 | 0.952717745058 | 0.381351379128 |
| 0.451683902792 | 0.956526168916 | 0.259525637381 |
| 0.362847314216 | 0.264774476226 | 0.442385947783 |
| 0.419024468194 | 0.230367907644 | 0.215582198180 |
| 0.470816786197 | 0.042219761142 | 0.408954450502 |
| 0.376444312778 | 0.098523231145 | 0.343761308538 |
| 0.287903414179 | 0.211996100420 | 0.349216917939 |
| 0.278176133537 | 0.282572917227 | 0.425256011624 |
| 0.174107248143 | 0.249616229571 | 0.315362239549 |
| 0.362437073718 | 0.012618986774 | 0.300024468857 |

Type A isomerisation, configuration P2 of the product

1.000000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1159301860450350 | 0.7531256657277994 | 0.2765325485996301 |
| 0.6152555370575646 | 0.2441006664903487 | 0.7784953798166679 |
| 0.8472347973578801 | 0.4756750097133354 | 0.3130889963310361 |
| 0.3392897603968190 | 0.9814279677245061 | 0.8230561514090821 |
| 0.8820418080886877 | 0.2072461739569292 | 0.0433192933042391 |
| 0.4002484383342499 | 0.6966981886920349 | 0.5530588635803195 |
| 0.7415464876851455 | 0.3743058734017451 | 0.2074822356022334 |
| 0.2388584083783698 | 0.8685616847390112 | 0.7126375294223306 |
| 0.0124707483867051 | 0.6427883536086183 | 0.1747545639497967 |
| 0.5067119386062092 | 0.1466853492056514 | 0.6654202863033851 |
| 0.2860972469639450 | 0.6017993658800654 | 0.4436661921929514 |
| 0.7824456202550490 | 0.0955066880007020 | 0.9424558011226143 |
| 0.2779019171355205 | 0.3770113956702500 | 0.6727739874337969 |
| 0.7823074481021539 | 0.8729503819974983 | 0.1714944768183808 |
| 0.7292236437257077 | 0.1524932843836170 | 0.4357751696255274 |
| 0.2387073612731102 | 0.6449966948160683 | 0.9412033338329041 |
| 0.3892649135510623 | 0.4729471072375081 | 0.7821794275594534 |
| 0.8880913780917457 | 0.9832562061245933 | 0.2730949437337334 |
| 0.1160806665700832 | 0.2077036701346582 | 0.8133645455858913 |
| 0.6148504370926048 | 0.7098158697873167 | 0.3149054273625192 |
| 0.3430205145927436 | 0.7546294327607868 | 0.0451697602672883 |
| 0.8364163921285894 | 0.2572429853685849 | 0.5466081092244099 |
| 0.5092189605634869 | 0.6065130202631576 | 0.2138903782443801 |
| 0.0164167298594129 | 0.0977967342488503 | 0.7037660467103665 |
| 0.2215885196726425 | 0.7917633239149229 | 0.1534733562833535 |
| 0.7222899684352404 | 0.2907201428248334 | 0.6622361595145984 |
| 0.2246365824038965 | 0.0928839361206948 | 0.8634158708394394 |
| 0.7286724036522119 | 0.5902111632738659 | 0.3306620548271676 |

| | | |
|--------------------|--------------------|--------------------|
| 0.9269899534898566 | 0.0925823431231869 | 0.1541707296377304 |
| 0.4368963640225597 | 0.5769730874211321 | 0.6623870718542233 |
| 0.6914562667774236 | 0.2673091524929050 | 0.3222532204758843 |
| 0.1984464198281661 | 0.7566289099932035 | 0.8290211052874659 |
| 0.3966163860469367 | 0.2679953579895515 | 0.6316830915269724 |
| 0.8997128507998000 | 0.7590417287361954 | 0.1408669697397678 |
| 0.4053396530524784 | 0.5586603334464807 | 0.3354141313009905 |
| 0.9028492841950113 | 0.0649051470871087 | 0.8368304059921157 |
| 0.1700644168593264 | 0.6830853571861725 | 0.3916983933880786 |
| 0.6605191161335037 | 0.1643992062423209 | 0.8977674454113713 |
| 0.4580620346623312 | 0.0286214576317511 | 0.7385878765888280 |
| 0.9689125652774138 | 0.5204728252523811 | 0.2454537563292519 |
| 0.8102796486853406 | 0.3296383024942531 | 0.0868946095702870 |
| 0.3346048611156758 | 0.8154466805489986 | 0.5992835865789053 |
| 0.4585137240371235 | 0.6733817000537569 | 0.0972961930874894 |
| 0.9612047125527936 | 0.1797382788702438 | 0.5785064103826086 |
| 0.1596687160376622 | 0.3303350020345247 | 0.7508312743978198 |
| 0.6603744197464531 | 0.8299030673597709 | 0.2498266555061376 |
| 0.8119854601235437 | 0.0321684139027408 | 0.3913073917733608 |
| 0.3147799980615852 | 0.5216093323732701 | 0.9007281268348160 |
| 0.0089742713503220 | 0.8752855432142770 | 0.2996769206666862 |
| 0.5049233254831902 | 0.3605621080068630 | 0.8121608835514759 |
| 0.8555915882877071 | 0.3844276708633972 | 0.4450747367493142 |
| 0.3707421062081384 | 0.8777671117543926 | 0.9445108390186199 |
| 0.9999317434981587 | 0.2295444309478355 | 0.9307200011048323 |
| 0.5234995381870854 | 0.7172610529001643 | 0.4474018243101616 |
| 0.6255525541235548 | 0.4919052462628991 | 0.1870361393262606 |
| 0.1257700874450297 | 0.9683249022379529 | 0.6705271330441922 |
| 0.1188246169717133 | 0.6213577153574320 | 0.0522490927840377 |
| 0.6058985870269074 | 0.1258843083135727 | 0.5383074835691547 |
| 0.2543446433198141 | 0.4817399142275094 | 0.5486285251273223 |
| 0.7573924362111147 | 0.9718723347771067 | 0.0479511268899658 |
| 0.0637510747233826 | 0.6623291029353178 | 0.2625503797005320 |
| 0.5665155367324163 | 0.1630026414728295 | 0.7469379606879801 |
| 0.8384400662254570 | 0.4082855812637389 | 0.2329692243792731 |
| 0.3128252156768345 | 0.9232685905474359 | 0.7474565597984586 |
| 0.7877375905968056 | 0.1811065305407230 | 0.0075668312418189 |
| 0.3126294777295611 | 0.6807102712108802 | 0.4988784007766189 |
| 0.0876065739729616 | 0.1848717333449684 | 0.7139166051784342 |
| 0.5466210003737946 | 0.7045402909814124 | 0.2334864756451440 |
| 0.3001903834946308 | 0.4301264355329581 | 0.7560356101082232 |
| 0.8027705082830535 | 0.9306008145721267 | 0.2524961296620496 |
| 0.3242369848843830 | 0.6733074277184784 | 0.9868842044856629 |
| 0.8043511302267460 | 0.1836069452844067 | 0.4897982960419525 |
| 0.1956472642185990 | 0.3713102779803368 | 0.4257885813134181 |
| 0.4598135270073906 | 0.2648590791639607 | 0.2210076267231895 |
| 0.5205516511939088 | 0.1339879589966617 | 0.1688656152152763 |
| 0.3813582622631380 | 0.2427102337856595 | 0.1446963801714441 |
| 0.5372944051854949 | 0.9905484130414327 | 0.3749826846112442 |
| 0.4875614237971411 | 0.1223566068939209 | 0.4206047571008042 |
| 0.4118927667484861 | 0.0077377561584511 | 0.5059564410626766 |
| 0.2090344069815828 | 0.2317745766700886 | 0.5398451975252483 |
| 0.0902457029218294 | 0.2000691683907360 | 0.4285386333027510 |
| 0.1637306521483809 | 0.2008137306034150 | 0.2723005151319479 |
| 0.1049230114019499 | 0.3377982627069180 | 0.3194899329472515 |
| 0.3057643346456039 | 0.0566414238743724 | 0.2370924767325746 |
| 0.2976032366394452 | 0.9669642446792699 | 0.3912940672676916 |
| 0.4400464143825115 | 0.9566580952136678 | 0.2755746400379719 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3439470635824212 | 0.2737618171674382 | 0.4448514736141977 |
| 0.4364027636323556 | 0.1974886176204269 | 0.2079766356513248 |
| 0.4566664076201071 | 0.0565849896624736 | 0.4141893873465782 |
| 0.3727790491508081 | 0.1156990003353140 | 0.3330232568874104 |
| 0.2618359602632889 | 0.2107705734668331 | 0.3712026094164030 |
| 0.2559540796030073 | 0.2780626699913970 | 0.4443528368733344 |
| 0.1533692972596389 | 0.2403727535165898 | 0.3394623910748645 |
| 0.3512083824986342 | 0.0186021818479678 | 0.3078708873089074 |

Type A isomerisation, configuration R3 of the reactant

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1268650597234863 | 0.7362006315619208 | 0.2753105926706458 |
| 0.6268185346495349 | 0.2243257751830678 | 0.7766261954585073 |
| 0.8581162188835180 | 0.4578476253046717 | 0.3130806228879111 |
| 0.3496820411077859 | 0.9632272391913110 | 0.8211495600112844 |
| 0.8933927583914324 | 0.1897357373150428 | 0.0424577797396127 |
| 0.4106313863311547 | 0.6787124706547539 | 0.5526047807539618 |
| 0.7527722544636256 | 0.3567697872262401 | 0.2061654033837340 |
| 0.2489093323225953 | 0.8499632028834482 | 0.7118582418186608 |
| 0.0226692672469279 | 0.6255391738540961 | 0.1732316880330305 |
| 0.5185989767538992 | 0.1278812882262664 | 0.6646716876179726 |
| 0.2972076225416640 | 0.5822670477033293 | 0.4426103658738267 |
| 0.7922057910966686 | 0.0790810691012744 | 0.9415904522788934 |
| 0.2879142669469058 | 0.3599058704011038 | 0.6718350918717301 |
| 0.7927579514876872 | 0.8558429767324287 | 0.1700081933651596 |
| 0.7387962299399713 | 0.1354282132980436 | 0.4342327888559475 |
| 0.2504543159341618 | 0.6256154149032812 | 0.9405819987335774 |
| 0.3988460609921881 | 0.4556505695682918 | 0.7803334180833189 |
| 0.8990059045635692 | 0.9658557055157813 | 0.2723063197068645 |
| 0.1263509045522412 | 0.1893908329686607 | 0.8121200108433272 |
| 0.6258340765254568 | 0.6927544490155657 | 0.3138579864547023 |
| 0.3539987873603199 | 0.7371217166314386 | 0.0442300917693852 |
| 0.8482659972971198 | 0.2386643901320272 | 0.5453193440954911 |
| 0.5206893918599611 | 0.5890919018329454 | 0.2124537112602626 |
| 0.0260889594984646 | 0.0810162229649621 | 0.7019153035578929 |
| 0.2330269033860935 | 0.7748067420269598 | 0.1526588324508718 |
| 0.7328506449078407 | 0.2726572339175322 | 0.6609527934868298 |
| 0.2349640643619739 | 0.0739474919160548 | 0.8622717973424413 |
| 0.7407171084292012 | 0.5740191453646586 | 0.3287801128775084 |
| 0.9378701158070161 | 0.0754513163443624 | 0.1539093325332587 |
| 0.4476299432682340 | 0.5613054883381479 | 0.6637988418770178 |
| 0.7016192830617231 | 0.2497005604078747 | 0.3197208294976226 |
| 0.2125192557034875 | 0.7347217914056825 | 0.8268066141641718 |
| 0.4097121798912316 | 0.2519251494311477 | 0.6350355319260029 |
| 0.9097450799327446 | 0.7409994675806073 | 0.1391489503428478 |
| 0.4164986737494339 | 0.5406290493122927 | 0.3333963838852566 |
| 0.9113819248490775 | 0.0489375302536639 | 0.8352471377941022 |
| 0.1814144926300595 | 0.6644688736828096 | 0.3902564199649313 |
| 0.6691806394065667 | 0.1494421797246291 | 0.8982384582729404 |
| 0.4679440657514029 | 0.0110017719147723 | 0.7360964608736752 |
| 0.9809379675405873 | 0.5018584249224018 | 0.2441839176983858 |
| 0.8219171516609208 | 0.3127063962989478 | 0.0853232602369189 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3435851490705450 | 0.7991334126055125 | 0.5963071945569763 |
| 0.4697008728474455 | 0.6557723500959541 | 0.0959993279487911 |
| 0.9721080345963224 | 0.1600961267766240 | 0.5766648409926770 |
| 0.1712418472254466 | 0.3113845654708218 | 0.7508930615771288 |
| 0.6705157809666701 | 0.8132934695791425 | 0.2493173725704286 |
| 0.8217640983459383 | 0.0145397816013240 | 0.3904978706714473 |
| 0.3276521946620038 | 0.5003407013844888 | 0.9024306728130501 |
| 0.0201043162106194 | 0.8579864829336857 | 0.2992493875258935 |
| 0.5122006513143720 | 0.3394802121995946 | 0.8083119509960153 |
| 0.8654519358225142 | 0.3674667805352488 | 0.4450455226201847 |
| 0.3820509025710081 | 0.8593191313706793 | 0.9424737839149409 |
| 0.0116720080637229 | 0.2117461520852991 | 0.9307840186069403 |
| 0.5335919170415674 | 0.6994078347276834 | 0.4463690028518520 |
| 0.6366318795666963 | 0.4743980845688298 | 0.1853980938109797 |
| 0.1330352495666689 | 0.9476854466941742 | 0.6751564019126468 |
| 0.1301809976084120 | 0.6015207425162080 | 0.0515079096316157 |
| 0.6146520402569012 | 0.1092617043204748 | 0.5355358723558949 |
| 0.2656908548221758 | 0.4608859549002662 | 0.5450459452425099 |
| 0.7675749986239669 | 0.9548353594817023 | 0.0467577227573407 |
| 0.0750931415286007 | 0.6461019424076131 | 0.2594040653708988 |
| 0.5828210412110504 | 0.1383194094942612 | 0.7462274929991901 |
| 0.8488605720837539 | 0.3910278853328039 | 0.2325743775141152 |
| 0.3239456937955827 | 0.9028983932788081 | 0.7471119329451891 |
| 0.7984978911142216 | 0.1634426780449722 | 0.0076446308404080 |
| 0.3242126929757825 | 0.6587953414152299 | 0.5000045218362118 |
| 0.0958788993208442 | 0.1674699005882968 | 0.7142291742438951 |
| 0.5578819079381151 | 0.6868098549706366 | 0.2324721210847719 |
| 0.3052342667958871 | 0.4207933887423531 | 0.7522313674401306 |
| 0.8152773140907372 | 0.9122715246452469 | 0.2505605557724627 |
| 0.3341422355351318 | 0.6534620832521869 | 0.9890242990413504 |
| 0.8129382356224637 | 0.1680230610133543 | 0.4876804878054860 |
| 0.3013914109009805 | 0.4480117585664484 | 0.2112152840382762 |
| 0.5087479148521752 | 0.0058905349225678 | 0.2998072546678624 |
| 0.4665351734893670 | 0.1054600341657741 | 0.1652003624005462 |
| 0.5271754058243683 | 0.1547680533978816 | 0.2370222517170388 |
| 0.4142618377934788 | 0.1760376947180680 | 0.4488569705388690 |
| 0.2648972621125354 | 0.1592821540515257 | 0.5257123833920345 |
| 0.3928234200477536 | 0.0305464232379167 | 0.5056626876739742 |
| 0.2435974850821883 | 0.3787486777147904 | 0.3711973508123643 |
| 0.1534895095576683 | 0.3497184499198235 | 0.2002875007142534 |
| 0.2468736059475829 | 0.2137712549120101 | 0.1565666568833497 |
| 0.2903188647173178 | 0.3535002540923017 | 0.0873957152428959 |
| 0.1718864218820807 | 0.0866509580562885 | 0.4184570036653913 |
| 0.3074560588295891 | 0.9645075006943137 | 0.4189243834829679 |
| 0.2693967717094404 | 0.0482018593623176 | 0.2807166062738241 |
| 0.3995985345146653 | 0.3391300958724528 | 0.3044796920901403 |
| 0.4699283534357945 | 0.1010868896735887 | 0.2522386430523214 |
| 0.3533672238578117 | 0.1268605123604956 | 0.4626962111412220 |
| 0.3381040092868921 | 0.1389545190532505 | 0.3440582631160402 |
| 0.2997809014860517 | 0.2630071987270666 | 0.2681267188925919 |
| 0.3135992700013682 | 0.3638364774182415 | 0.2855329957246032 |
| 0.2484271548994795 | 0.2919051306771354 | 0.1719699907028188 |
| 0.2667257532471722 | 0.0553742897838304 | 0.3653901404854104 |

Type A isomerization, configuration TS3 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |

| | | |
|----------------|----------------|----------------|
| 3.961547000001 | 6.862197999978 | 9.876069999981 |
| Si Al O H C | | |
| 23 1 48 15 7 | | |
| direct | | |
| 0.125732803988 | 0.734514564252 | 0.276440898873 |
| 0.626184886669 | 0.224616472244 | 0.778339791734 |
| 0.856414033808 | 0.458395986600 | 0.313700898996 |
| 0.348708335597 | 0.963135509525 | 0.823434122612 |
| 0.892341893333 | 0.188569867587 | 0.043991439711 |
| 0.409675918426 | 0.679578310489 | 0.552300592205 |
| 0.750687950021 | 0.355906322537 | 0.207898078284 |
| 0.248149660196 | 0.850730900623 | 0.712784646230 |
| 0.022666497220 | 0.623235199937 | 0.174329994143 |
| 0.517010367011 | 0.128149369498 | 0.666075823951 |
| 0.295133011191 | 0.583116645051 | 0.444555591091 |
| 0.792309438479 | 0.078613731902 | 0.941485119140 |
| 0.287295244307 | 0.359488471750 | 0.673406196916 |
| 0.791882763148 | 0.855528411313 | 0.170414477494 |
| 0.738455039479 | 0.134208059452 | 0.436199581795 |
| 0.248005486440 | 0.626842335566 | 0.940815279725 |
| 0.400003804041 | 0.456172476047 | 0.780023670435 |
| 0.896777012165 | 0.964919533494 | 0.273528781566 |
| 0.125870201580 | 0.189399316101 | 0.813651016324 |
| 0.624653805948 | 0.693639633128 | 0.312671974957 |
| 0.351659976355 | 0.737306944793 | 0.046007694384 |
| 0.848092881761 | 0.238451897398 | 0.545951869246 |
| 0.518787751699 | 0.587906406196 | 0.213840988156 |
| 0.026490593624 | 0.082699751040 | 0.700859350875 |
| 0.231199950133 | 0.776014257251 | 0.154402480344 |
| 0.734082484767 | 0.269988156321 | 0.663443460900 |
| 0.234042375047 | 0.073919022425 | 0.864566176606 |
| 0.740165584959 | 0.576032578701 | 0.328651238450 |
| 0.937162485561 | 0.073934320658 | 0.155105453149 |
| 0.448611669916 | 0.560432585206 | 0.661288727727 |
| 0.700596718308 | 0.248351704697 | 0.321911339630 |
| 0.209243003551 | 0.736893787126 | 0.827631359173 |
| 0.407801680379 | 0.251103741530 | 0.634333481677 |
| 0.909125668450 | 0.740009693832 | 0.143333104927 |
| 0.415103537831 | 0.541057713519 | 0.336169901236 |
| 0.910583054009 | 0.051790154481 | 0.833304576038 |
| 0.179600653789 | 0.664609160965 | 0.391777355038 |
| 0.667550453108 | 0.148105910757 | 0.900693142189 |
| 0.467094993158 | 0.010803485534 | 0.738336583904 |
| 0.979999804214 | 0.500441386710 | 0.245106710959 |
| 0.820372967500 | 0.311157560736 | 0.087401371218 |
| 0.344231134840 | 0.798702429424 | 0.598269314426 |
| 0.467010846781 | 0.653858633501 | 0.097935810170 |
| 0.973538140518 | 0.161897613702 | 0.574837694812 |
| 0.170338015397 | 0.311495435975 | 0.753726245563 |
| 0.667888655617 | 0.815315199512 | 0.246927198460 |
| 0.821001721664 | 0.013553867624 | 0.391917078505 |
| 0.328070628817 | 0.503530263053 | 0.900070618540 |
| 0.016423137939 | 0.854887172792 | 0.300519351819 |
| 0.514057167159 | 0.341444644108 | 0.809902603817 |
| 0.860974915144 | 0.368527033383 | 0.446508395479 |
| 0.381272657560 | 0.859178845923 | 0.944589298658 |
| 0.010027676408 | 0.211041604625 | 0.931706369336 |
| 0.531338836864 | 0.701766648592 | 0.444487942374 |

| | | |
|----------------|----------------|----------------|
| 0.633605372996 | 0.472255347756 | 0.186991094180 |
| 0.133898705996 | 0.949659553241 | 0.673347649180 |
| 0.127639411874 | 0.601557962166 | 0.050536199499 |
| 0.614392345946 | 0.108039614935 | 0.537885334315 |
| 0.264022462018 | 0.462329074369 | 0.548180344379 |
| 0.770563295190 | 0.952680514508 | 0.044900252121 |
| 0.078043881353 | 0.642024471653 | 0.259317181082 |
| 0.579145033491 | 0.141186698238 | 0.747831881227 |
| 0.845636798181 | 0.391999714386 | 0.233740178044 |
| 0.322720739275 | 0.903453700791 | 0.748925256761 |
| 0.797327653672 | 0.162172494124 | 0.009257319934 |
| 0.321066105164 | 0.661706253496 | 0.500778274850 |
| 0.097338257702 | 0.167396326456 | 0.714410624044 |
| 0.558056658620 | 0.685806853586 | 0.231225244981 |
| 0.307855162501 | 0.417268996518 | 0.754270561918 |
| 0.810335336666 | 0.914689840655 | 0.251492432768 |
| 0.330449032730 | 0.655721832429 | 0.989756622619 |
| 0.813058848899 | 0.166254298308 | 0.489615599449 |
| 0.396506215625 | 0.403874611973 | 0.156454171648 |
| 0.491411413535 | 0.027264594489 | 0.267553820211 |
| 0.484732122439 | 0.154740921137 | 0.138414013672 |
| 0.533162883031 | 0.153630016821 | 0.256101934146 |
| 0.406984774618 | 0.186478711839 | 0.450322171016 |
| 0.265479952261 | 0.153347379663 | 0.531675343447 |
| 0.400676024152 | 0.034062111427 | 0.503432975804 |
| 0.263765329000 | 0.422231587644 | 0.280547480391 |
| 0.170780388127 | 0.334398226744 | 0.192343880580 |
| 0.262585477205 | 0.199446411498 | 0.149861037235 |
| 0.307906527227 | 0.335704735592 | 0.073017164921 |
| 0.172185078121 | 0.085258857845 | 0.423913349437 |
| 0.307978265533 | 0.964552959193 | 0.425813511542 |
| 0.269576824818 | 0.047902439600 | 0.286518668964 |
| 0.406170129939 | 0.336191459059 | 0.309077432700 |
| 0.473834091476 | 0.126275357572 | 0.235999617797 |
| 0.354080103576 | 0.129289926561 | 0.464400932052 |
| 0.329681356091 | 0.143026419937 | 0.351907136432 |
| 0.325048111460 | 0.251353659839 | 0.253767287868 |
| 0.352300741386 | 0.357702615509 | 0.250006297175 |
| 0.265231455653 | 0.279530727573 | 0.160959599164 |
| 0.267617171848 | 0.054662377373 | 0.370909879050 |

Type A isomerisation, configuration P3 of the product

1.000000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.961560999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1263762350249971 | 0.7350246411834962 | 0.2760351029840424 |
| 0.6299380840660410 | 0.2258548629994547 | 0.7752171873307633 |
| 0.8585986081716230 | 0.4579383069180478 | 0.3142935082151285 |
| 0.3512272674718698 | 0.9625775552517614 | 0.8229352810895417 |
| 0.8933191674518282 | 0.1882130440157748 | 0.0440752133406078 |
| 0.4081185593209544 | 0.6831757680679739 | 0.5507331218657137 |
| 0.7520535974695153 | 0.3563488010617985 | 0.2067239000212808 |
| 0.2503783235192722 | 0.8486549458626017 | 0.7149370165397281 |
| 0.0242171479407879 | 0.6239533252789284 | 0.1723170198807176 |

0.5182346485265632 0.1287525633741463 0.6650562526788087
0.2962518956460065 0.5830011063268302 0.4440477652436480
0.7909314148842947 0.0801730597213746 0.9434264960359137
0.2890885859366734 0.3590893952331120 0.6736811022694059
0.7954049586594621 0.8534217283579187 0.1674949092069699
0.7407925444641890 0.1321550034444260 0.4352049466712699
0.2538458235805438 0.6230030836079217 0.9421252512511369
0.4029834361558744 0.4568561080578605 0.7790629166744115
0.8999105642491380 0.9635953514662625 0.2721573307910366
0.1273967075652518 0.1898645986411699 0.8124426536207959
0.6282802175866349 0.6904449250655589 0.3159359924142327
0.3541353073893392 0.7367339915394369 0.0461215331812548
0.8538122996900609 0.2330664846038757 0.5436109261889136
0.5212079391272082 0.5857218359994076 0.2146538668440188
0.0272215802148334 0.0817380011677029 0.7045706706853295
0.2318170899762496 0.7746294492325668 0.1530825544080604
0.7412510339573257 0.2659278166417327 0.6607253476556887
0.2353373136355027 0.0734832821853920 0.8622437705320742
0.7408889152394066 0.5713801736859193 0.3413162234980787
0.9392226906188772 0.0738310298059998 0.1546075122782896
0.4445305639424401 0.5659583815713259 0.6620278327575141
0.7049585993346984 0.2481100005302392 0.3218575597173438
0.2161042660444087 0.7323423928550012 0.8277314090164668
0.4074997039294762 0.2498115904323838 0.6329125640592013
0.9125539429740662 0.7397286060990861 0.1345714592554188
0.4169395293899493 0.5400705749875435 0.3369566193202623
0.9105862450237147 0.0551175154743026 0.8356073877883784
0.1810454490564169 0.6627254801633174 0.3907392506245958
0.6687328316331898 0.1499629444428172 0.8987798788143800
0.4695240369936152 0.0105992913360182 0.7388009237334054
0.9804909641007926 0.5020487643831054 0.2441847064300995
0.8247572039372116 0.3111350332219649 0.0866017595704323
0.3409702817639985 0.8040243226662895 0.5945717150892756
0.4687708155546225 0.6570976489067425 0.0992866362799215
0.9793414850205346 0.1553385392762749 0.5742777886484658
0.1713865060316958 0.3119420601809915 0.7546946288424824
0.6737684499069738 0.8103849997377420 0.2469728472041568
0.8198755392136292 0.0115371816460847 0.3906227168970212
0.3322859076202410 0.4993499473136624 0.9019474812807247
0.0208153077427877 0.8572471569449593 0.3011499239791411
0.5221917978022849 0.3465449667237117 0.8017584656613136
0.8720151879528322 0.3601645034646265 0.4421974076078057
0.3820950456416744 0.8594496878153955 0.9447765820735362
0.0102093974102861 0.2091425396644321 0.9296490263576525
0.5306624916998307 0.7043843035164512 0.4445302745034954
0.6328586279664880 0.4690699080164643 0.1850837192769522
0.1329321237514509 0.9470720582474308 0.6815910553292887
0.1331908783557978 0.5996400779259904 0.0517402079695153
0.6160050480118439 0.1084761423953522 0.5372029341114283
0.2648358947505190 0.4632109396608398 0.5496156204241343
0.7692914127448303 0.9535820044396009 0.0447600878326114
0.0728546261508725 0.6469882653513779 0.2598440714590867
0.5795776918326111 0.1446241977851749 0.7455955672899911
0.8435241874934559 0.3980011929617012 0.2314940278449421
0.3272120549213848 0.9020709300502017 0.7474367351027236
0.7955672231163390 0.1627814689756097 0.0123363742201538
0.3207728046805491 0.6640553332282051 0.4987411319158137
0.0999509154654962 0.1697500137501051 0.7106430305484768

| | | |
|--------------------|--------------------|--------------------|
| 0.5660872482337586 | 0.6784477121719030 | 0.2333047495841369 |
| 0.3129495664943351 | 0.4138034706091654 | 0.7547615521228477 |
| 0.8189543267725864 | 0.9091705964053884 | 0.2478996602578976 |
| 0.3371276852134359 | 0.6531153758826685 | 0.9889017453594097 |
| 0.8191955611301346 | 0.1591942870858763 | 0.4891340573674146 |
| 0.3556924007625301 | 0.4130287508600706 | 0.1719204848447477 |
| 0.4690768523506923 | 0.0796305702084776 | 0.1936252796221083 |
| 0.4910247152735049 | 0.2251655736115449 | 0.1072041381095497 |
| 0.5176215890665588 | 0.1529785582871616 | 0.2529009781698657 |
| 0.3963199753392451 | 0.1783145186375917 | 0.4488577671732676 |
| 0.2483220847911309 | 0.1636257009396502 | 0.5421744570538994 |
| 0.3653770699947155 | 0.0327251515592880 | 0.5182021390544560 |
| 0.2280090225227078 | 0.4061421688984916 | 0.3042462880338788 |
| 0.1552525867008849 | 0.3070868877425574 | 0.2057409233208917 |
| 0.2668704081902138 | 0.1881195292689166 | 0.1424777386903400 |
| 0.2843865143060577 | 0.3354543163624101 | 0.0823764183158642 |
| 0.1267884397703142 | 0.1182399130328809 | 0.4444222661161041 |
| 0.2426483735067912 | 0.9822730401905231 | 0.4568015712506351 |
| 0.2116031843331157 | 0.0709448989568037 | 0.3099179065333769 |
| 0.3785168172989562 | 0.3411558873336401 | 0.3175145555280981 |
| 0.4603173854602242 | 0.1671897817564491 | 0.1997755394443049 |
| 0.3317926203402312 | 0.1297863544557405 | 0.4721236282914524 |
| 0.2921484222832486 | 0.1470752913315010 | 0.3710650106701511 |
| 0.3241048947283526 | 0.2382544333252863 | 0.2530370163357290 |
| 0.3214253541846795 | 0.3562617203973353 | 0.2638513671582328 |
| 0.2528021978999958 | 0.2679897896439395 | 0.1666065027110095 |
| 0.2208989290573308 | 0.0722219251357648 | 0.3915474263138825 |

Type A isomerisation, configuration R4 of the reactant

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.862258999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.876069999810004 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1089486358570307 | 0.7530821630626688 | 0.2804447070906048 |
| 0.6094119770300371 | 0.2452751789178799 | 0.7799336112166890 |
| 0.8430649989354345 | 0.4748791169898074 | 0.3151159005246771 |
| 0.3331643846554355 | 0.9811192474624723 | 0.8267821236192364 |
| 0.8772894156839816 | 0.2072204380890750 | 0.0477438948410426 |
| 0.3924535074497074 | 0.6965621694459831 | 0.5576575101638724 |
| 0.7342817217232651 | 0.3742541394988387 | 0.2120212060378150 |
| 0.2345217044921036 | 0.8683962150707006 | 0.7144454946355379 |
| 0.0046997879198386 | 0.6443319676107242 | 0.1770293617897765 |
| 0.5009594364837973 | 0.1460994534400819 | 0.6699544123931407 |
| 0.2786807551588586 | 0.6015919493598522 | 0.4480510986244664 |
| 0.7766858295047816 | 0.0935447204671549 | 0.9453338194541088 |
| 0.2703273479499069 | 0.3766822488852005 | 0.6772489428326693 |
| 0.7731778542808466 | 0.8734254692811012 | 0.1778636038941214 |
| 0.7220756601772177 | 0.1527054904381606 | 0.4410514518209767 |
| 0.2329918145161126 | 0.6441003056733723 | 0.9446663671545854 |
| 0.3791860343035378 | 0.4724247829197951 | 0.7881212279408016 |
| 0.8807315445826185 | 0.9825664019280236 | 0.2791718921671260 |
| 0.1083557864594330 | 0.2066075443348196 | 0.8206335421739525 |
| 0.6086896978122439 | 0.7081285265425507 | 0.3196403078651449 |
| 0.3361343711628552 | 0.7543564326943546 | 0.0494442090281360 |
| 0.8310254559627598 | 0.2576906903090023 | 0.5502850875144233 |

| | | |
|--------------------|--------------------|--------------------|
| 0.5021935313901215 | 0.6069158854144651 | 0.2181289518159605 |
| 0.0073665303743099 | 0.0942703739851164 | 0.7104492807470976 |
| 0.2150187183662544 | 0.7921561531680759 | 0.1578229892035274 |
| 0.7140374200343338 | 0.2948922825344304 | 0.6636836530748600 |
| 0.2193058970564135 | 0.0924774857498350 | 0.8677182427420769 |
| 0.7248209045766869 | 0.5907285497072751 | 0.3313614843896348 |
| 0.9179789522959683 | 0.0922334929259930 | 0.1602912857573741 |
| 0.4250915910105551 | 0.5786923080980679 | 0.6700882772985014 |
| 0.6843049344615093 | 0.2672854801323166 | 0.3271242912130936 |
| 0.1989884169467042 | 0.7525310568936775 | 0.8282500450798050 |
| 0.3916309675868778 | 0.2687243799631365 | 0.6386624414752252 |
| 0.8901903483381091 | 0.7605133368430564 | 0.1449904912383104 |
| 0.3982466256134867 | 0.5594897304263794 | 0.3394144132891658 |
| 0.8938626207367638 | 0.0530485485597413 | 0.8420166310787275 |
| 0.1627533332282046 | 0.6823205127318099 | 0.3957584529470524 |
| 0.6543221964684596 | 0.1682406769118685 | 0.9005676021495462 |
| 0.4522323288101193 | 0.0281215365338644 | 0.7431927538255781 |
| 0.9639107746255779 | 0.5206852442472844 | 0.2460173332080028 |
| 0.7992811532262184 | 0.3288149758721033 | 0.0919801988560658 |
| 0.3302078796364097 | 0.8188635454908170 | 0.5982414168565977 |
| 0.4519163729526038 | 0.6734774875614982 | 0.1013154930138299 |
| 0.9523882262499691 | 0.1789932460007483 | 0.5862937012502544 |
| 0.1530224482230410 | 0.3286976392514455 | 0.7525104279092198 |
| 0.6503557094596705 | 0.8311164281702389 | 0.2565002798355658 |
| 0.8041512836474622 | 0.0318525254848176 | 0.3969893094667630 |
| 0.3077770505074369 | 0.5176059249996233 | 0.9092158266035856 |
| 0.0020396958558586 | 0.8751642933959712 | 0.3045338916252942 |
| 0.4954546273969788 | 0.3589245033463068 | 0.8152669688811229 |
| 0.8507892021070583 | 0.3840867304375863 | 0.4471280522194063 |
| 0.3644329776433992 | 0.8769825161662167 | 0.9483171061630786 |
| 0.9980013849671900 | 0.2313278614954297 | 0.9416721487660605 |
| 0.5182751519473622 | 0.7112496603080564 | 0.4532751739838343 |
| 0.6181173576100506 | 0.4917854684832861 | 0.1921159691813522 |
| 0.1186570525533407 | 0.9658029643297404 | 0.6769659430613442 |
| 0.1097509636301630 | 0.6263614621859870 | 0.0528610144722249 |
| 0.5978464907905231 | 0.1259608799606975 | 0.5415477935859531 |
| 0.2485842972843819 | 0.4809826359146762 | 0.5524578016895461 |
| 0.7430047689931236 | 0.9760982584069479 | 0.0574045490999993 |
| 0.0559449477615712 | 0.6644665924583106 | 0.2643633050402272 |
| 0.5644492317604453 | 0.1594653968424505 | 0.7504595332098275 |
| 0.8324767581558425 | 0.4079047663909164 | 0.2354600617474878 |
| 0.3074333707700173 | 0.9228844292118872 | 0.7508280319543087 |
| 0.7886524012452789 | 0.1800243912662514 | 0.0049677225161987 |
| 0.3047124256872664 | 0.6811808036127882 | 0.5031185368550943 |
| 0.0699572882464925 | 0.1811470452389244 | 0.7309707065136916 |
| 0.5402528436583122 | 0.7050632455856226 | 0.2369858644253235 |
| 0.2884933620922001 | 0.4316577407022972 | 0.7621486437645049 |
| 0.7944956792202092 | 0.9298507389533907 | 0.2594737753731189 |
| 0.3171790118344045 | 0.6720322237611541 | 0.9924374666643535 |
| 0.7965683952167222 | 0.1840696303923046 | 0.4950117963717385 |
| 0.3595670202699128 | 0.0678355915642452 | 0.5152834584271919 |
| 0.1584742436725227 | 0.3295896874644250 | 0.3432600893776376 |
| 0.3019647912019106 | 0.3608245990829868 | 0.2665037108692027 |
| 0.2399821300505516 | 0.3132537190902513 | 0.1942388937353987 |
| 0.5991047191346804 | 0.1680945376039628 | 0.1753772024745631 |
| 0.5041274328493490 | 0.2294493368805043 | 0.3027697918479994 |
| 0.5643414911991526 | 0.0729358768723439 | 0.3281764807978741 |
| 0.3582399207646330 | 0.2229123470195315 | 0.4581792416606781 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2029196844808815 | 0.1056730260315188 | 0.2902261369738300 |
| 0.1346492933030866 | 0.1230826207259371 | 0.4382880007111923 |
| 0.2612761171737532 | 0.9954292833160006 | 0.4131744427776121 |
| 0.3551925986811475 | 0.1024828572212628 | 0.1490742180824002 |
| 0.5000095742082186 | 0.0090507895330328 | 0.1729080125582028 |
| 0.4922755271321875 | 0.1519605062251718 | 0.0698322303679567 |
| 0.2196736620175100 | 0.1853371821456939 | 0.5301547478122643 |
| 0.2493880940123446 | 0.3029276501931804 | 0.2807192555819494 |
| 0.5275103524401199 | 0.1579647142813967 | 0.2621559574432110 |
| 0.4214697327067869 | 0.1422376502817155 | 0.2570317761493948 |
| 0.3047798867344761 | 0.1648356537646385 | 0.3501908648952554 |
| 0.3120285395120578 | 0.1602485821649336 | 0.4699421774735457 |
| 0.2215691852347549 | 0.0925358872663003 | 0.3728981691621758 |
| 0.4379749594331628 | 0.1034938128869229 | 0.1561168658978149 |

Type A isomerization, configuration TS4 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

Si Al O H C

23 1 48 15 7

direct

| | | |
|------------|------------|------------|
| 0.11247096 | 0.75339760 | 0.28490746 |
| 0.61284871 | 0.24667005 | 0.78557252 |
| 0.84649170 | 0.47575088 | 0.31804243 |
| 0.33691859 | 0.98225081 | 0.83219038 |
| 0.88105235 | 0.20717950 | 0.05244156 |
| 0.39619165 | 0.69889512 | 0.56073128 |
| 0.73784238 | 0.37410678 | 0.21681831 |
| 0.23890395 | 0.87032350 | 0.71773495 |
| 0.00840510 | 0.64426104 | 0.18119942 |
| 0.50374579 | 0.14750044 | 0.67531056 |
| 0.28179459 | 0.60373498 | 0.45304005 |
| 0.78120472 | 0.09353062 | 0.94830761 |
| 0.27481502 | 0.37667338 | 0.68217136 |
| 0.77647672 | 0.87425898 | 0.18098207 |
| 0.72744171 | 0.15218775 | 0.44594955 |
| 0.23553437 | 0.64612339 | 0.94812042 |
| 0.38434243 | 0.47347982 | 0.79241778 |
| 0.88373575 | 0.98325507 | 0.28306907 |
| 0.11258101 | 0.20755079 | 0.82593786 |
| 0.61229964 | 0.70967898 | 0.32233133 |
| 0.33935819 | 0.75514582 | 0.05446388 |
| 0.83584236 | 0.25796106 | 0.55358062 |
| 0.50545155 | 0.60723094 | 0.22310703 |
| 0.01256812 | 0.09672746 | 0.71257621 |
| 0.21892818 | 0.79384900 | 0.16315781 |
| 0.71864305 | 0.29218059 | 0.66774976 |
| 0.22362905 | 0.09378506 | 0.87391404 |
| 0.72922177 | 0.59254762 | 0.33178257 |
| 0.92292179 | 0.09314723 | 0.16527782 |
| 0.42652187 | 0.58096050 | 0.67395282 |
| 0.68904849 | 0.26770168 | 0.33318770 |
| 0.20266866 | 0.75400614 | 0.83084005 |
| 0.39410934 | 0.26853220 | 0.64080113 |
| 0.89300663 | 0.75930476 | 0.15126510 |
| 0.40148345 | 0.56085685 | 0.34505005 |

| | | |
|------------|------------|------------|
| 0.89682678 | 0.05630683 | 0.84176780 |
| 0.16564776 | 0.68285189 | 0.40067473 |
| 0.65739411 | 0.16868618 | 0.90598806 |
| 0.45622060 | 0.02865033 | 0.74869506 |
| 0.96927452 | 0.51919356 | 0.25030423 |
| 0.80168492 | 0.32872914 | 0.09673258 |
| 0.33544254 | 0.82124428 | 0.60134911 |
| 0.45487476 | 0.67231016 | 0.10633825 |
| 0.95922417 | 0.18328273 | 0.58709321 |
| 0.15658400 | 0.33014135 | 0.75830923 |
| 0.65345683 | 0.83258979 | 0.25945592 |
| 0.80787590 | 0.03134657 | 0.40157425 |
| 0.31097194 | 0.51879484 | 0.91375093 |
| 0.00489915 | 0.87506691 | 0.30884359 |
| 0.50284256 | 0.36360360 | 0.81983799 |
| 0.85151190 | 0.38598059 | 0.45106091 |
| 0.36833789 | 0.87774632 | 0.95374584 |
| 0.00206438 | 0.23239724 | 0.94693858 |
| 0.52309238 | 0.71026560 | 0.45706571 |
| 0.62195803 | 0.49238523 | 0.19784121 |
| 0.12399919 | 0.96813128 | 0.67803052 |
| 0.11224988 | 0.62713185 | 0.05581202 |
| 0.60476006 | 0.12602774 | 0.54958415 |
| 0.25180582 | 0.48426550 | 0.55962820 |
| 0.75041329 | 0.97378000 | 0.05782890 |
| 0.06172321 | 0.66407327 | 0.26704182 |
| 0.56105556 | 0.16435442 | 0.75914337 |
| 0.83783388 | 0.40795870 | 0.23790227 |
| 0.30972522 | 0.92455790 | 0.75678100 |
| 0.79510982 | 0.17806505 | 0.00850339 |
| 0.30696031 | 0.68607222 | 0.50590357 |
| 0.07585494 | 0.18092038 | 0.73590034 |
| 0.54264593 | 0.70700591 | 0.24044875 |
| 0.29663976 | 0.42690257 | 0.76879318 |
| 0.79832325 | 0.93201913 | 0.26087126 |
| 0.31830366 | 0.67462124 | 0.99701599 |
| 0.80631737 | 0.18139111 | 0.49738531 |
| 0.29191586 | 0.11927570 | 0.48296999 |
| 0.15744237 | 0.31937288 | 0.24460925 |
| 0.28487785 | 0.31772594 | 0.11553478 |
| 0.18787547 | 0.22732178 | 0.15039862 |
| 0.51167008 | 0.22166613 | 0.09684858 |
| 0.43379808 | 0.26569154 | 0.23404681 |
| 0.53348142 | 0.11703638 | 0.23714312 |
| 0.28934190 | 0.26753013 | 0.38113545 |
| 0.19002589 | 0.02875252 | 0.29416967 |
| 0.09269807 | 0.10555838 | 0.40806903 |
| 0.21882094 | 0.98159691 | 0.43648929 |
| 0.33232673 | 0.03162172 | 0.14407804 |
| 0.47742082 | 0.97991013 | 0.16756077 |
| 0.44687890 | 0.10604777 | 0.04279749 |
| 0.15175918 | 0.22500238 | 0.46314274 |
| 0.22691872 | 0.26195548 | 0.18730503 |
| 0.46566754 | 0.19187241 | 0.19425998 |
| 0.36823709 | 0.14014273 | 0.21610291 |
| 0.26475609 | 0.14237176 | 0.31974105 |
| 0.24857295 | 0.19392602 | 0.41558329 |
| 0.18683468 | 0.06054593 | 0.36417851 |

0.40537283 0.06102187 0.13781383

Type A isomerisation, configuration P4 of the product

1.000000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| | | | | |
|----|----|----|----|---|
| Si | Al | O | H | C |
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1166090272713065 | 0.7550204781164700 | 0.2854231287797613 |
| 0.6193796118941535 | 0.2528969188826155 | 0.7850032113813856 |
| 0.8526188895569073 | 0.4774303081255760 | 0.3173260371757911 |
| 0.3438229522641857 | 0.9855155212244534 | 0.8328696710814388 |
| 0.8900767276788613 | 0.2093230005114702 | 0.0533007195150639 |
| 0.3979221709834956 | 0.7042508217772999 | 0.5586927292994400 |
| 0.7422975440766835 | 0.3756456229174819 | 0.2182008907052891 |
| 0.2459150368916003 | 0.8743234079978357 | 0.7182522640565022 |
| 0.0114753408770533 | 0.6493937966636985 | 0.1788465917243164 |
| 0.5103129540873504 | 0.1507835502444770 | 0.6773667367371011 |
| 0.2864489988760498 | 0.6090613746732686 | 0.4529267412500952 |
| 0.7865113938778641 | 0.0953413302465790 | 0.9485410529937808 |
| 0.2816632128607625 | 0.3774040113558211 | 0.6841008154423958 |
| 0.7810524986605492 | 0.8772415408398913 | 0.1812004997927872 |
| 0.7349037451589233 | 0.1529543051800540 | 0.4476811959407267 |
| 0.2415160308823755 | 0.6497250481633990 | 0.9479740163835539 |
| 0.3879392663588568 | 0.4750624712583609 | 0.7931085221212838 |
| 0.8906063521853045 | 0.9848528181805534 | 0.2839810430016229 |
| 0.1172193306363773 | 0.2106060199678931 | 0.8298331538308086 |
| 0.6184515340974737 | 0.7105038593534370 | 0.3242840840654566 |
| 0.3453275729147529 | 0.7567558705683120 | 0.0550178286606612 |
| 0.8439320761876442 | 0.2589764423616129 | 0.5527902817385596 |
| 0.5112603976738864 | 0.6096088775982486 | 0.2240422185685703 |
| 0.0145028609906143 | 0.0965599794719387 | 0.7187907857986836 |
| 0.2240377304868668 | 0.7936304604368318 | 0.1639776489561928 |
| 0.7258053045537456 | 0.2949124124779703 | 0.6648849287080766 |
| 0.2308387453049090 | 0.0977051771826411 | 0.8736678005069767 |
| 0.7331362075878998 | 0.5911189286163399 | 0.3371914770573622 |
| 0.9301179982492307 | 0.0957687468678462 | 0.1676598145843598 |
| 0.4209797449105039 | 0.5829261445324490 | 0.6703521226644181 |
| 0.6955761556640643 | 0.2693574345158917 | 0.3362742487667634 |
| 0.2078924473090840 | 0.7598028816712528 | 0.8318562979177547 |
| 0.4006213517392060 | 0.2704695672771613 | 0.6396784809354275 |
| 0.8971198834387788 | 0.7640404600786697 | 0.1454150839635911 |
| 0.4066582040844166 | 0.5650021048159882 | 0.3464170377314267 |
| 0.8983870474026744 | 0.0499582972596228 | 0.8425799213002606 |
| 0.1692764553688130 | 0.6810823192636900 | 0.4015332276025748 |
| 0.6645382948503201 | 0.1773934002076601 | 0.9048792992222277 |
| 0.4637101610929977 | 0.0312769011264459 | 0.7519797152488326 |
| 0.9728298294071166 | 0.5244028084977742 | 0.2472498403413154 |
| 0.8045815703412510 | 0.3292685484631437 | 0.0987899479831901 |
| 0.3410890007192090 | 0.8248628210277984 | 0.6017970848517055 |
| 0.4605896247797642 | 0.6754960158521698 | 0.1073237048921611 |
| 0.9660717108903425 | 0.1842169408997359 | 0.5898581185454767 |
| 0.1620757289045696 | 0.3323850119571442 | 0.7527980214750759 |
| 0.6608800172384257 | 0.8321431837280924 | 0.2637542105990586 |
| 0.8133533574253379 | 0.0320742299978051 | 0.4028988865269607 |
| 0.3154756850426786 | 0.5239951818675158 | 0.9115912053779681 |

| | | |
|--------------------|--------------------|--------------------|
| 0.0134498279301453 | 0.8791117431041062 | 0.3101751886044101 |
| 0.5123206166176304 | 0.3730946166181035 | 0.8146335746549862 |
| 0.8636126788840082 | 0.3844759906199512 | 0.4480145920046414 |
| 0.3726331883086083 | 0.8802498674441201 | 0.9549232534333980 |
| 0.0128901069321957 | 0.2381607196228999 | 0.9534144876472045 |
| 0.5270153879616705 | 0.7116093403969175 | 0.4582901650150980 |
| 0.6259614489369293 | 0.4932880026593389 | 0.1997719596593510 |
| 0.1315289908141654 | 0.9733357864357557 | 0.6773628993402554 |
| 0.1181048453524957 | 0.6319581985032500 | 0.0553455783192010 |
| 0.6133887321555785 | 0.1272441360408219 | 0.5534105760056778 |
| 0.2608994353213215 | 0.4915012542819810 | 0.5650201259476688 |
| 0.7497275179664139 | 0.9805063254237401 | 0.0618685792666145 |
| 0.0602651665527238 | 0.6710643830961552 | 0.2672630369268864 |
| 0.5645498308648011 | 0.1710035621559938 | 0.7614749768921436 |
| 0.8429350913959137 | 0.4108787780612731 | 0.2366664701652539 |
| 0.3173757530548731 | 0.9293512717367771 | 0.7554220804848317 |
| 0.8133791457122234 | 0.1769268946310990 | 0.0018027693511729 |
| 0.3072492407276108 | 0.7015769164889786 | 0.4976920171844391 |
| 0.0706629324571705 | 0.1806891807183015 | 0.7499317099009838 |
| 0.5504580309039886 | 0.7085049778709921 | 0.2404051918853429 |
| 0.3024704440460431 | 0.4175123412702790 | 0.7793789297307403 |
| 0.8092659968315792 | 0.9308739523474991 | 0.2602126957945514 |
| 0.3261268708972574 | 0.6762967018360831 | 0.9962683641641125 |
| 0.8178583430004119 | 0.1794848440989734 | 0.4969610306915473 |
| 0.2445679153714995 | 0.0860307968842147 | 0.4885949639166585 |
| 0.1344323112296378 | 0.3134091257984616 | 0.1937152286511027 |
| 0.1986944781354734 | 0.2686852364509526 | 0.0581564227485580 |
| 0.0874108817491892 | 0.2032931938398697 | 0.1818814526703951 |
| 0.4164068610085149 | 0.2046216694631024 | 0.0550938811532049 |
| 0.3547176508490971 | 0.2683839967789755 | 0.1764437327877849 |
| 0.4562373003506743 | 0.1174403732678470 | 0.1917242899001519 |
| 0.2789414418041886 | 0.2183934202293905 | 0.3638236872389401 |
| 0.1106483655187264 | 0.0050109529536297 | 0.3325562243683365 |
| 0.0824061620038847 | 0.0248970102680179 | 0.4783386938193460 |
| 0.2168055288527652 | 0.9223861397018628 | 0.4150936659998025 |
| 0.2343358701807111 | 0.9988825466168315 | 0.1625069044686662 |
| 0.3835749213588042 | 0.9529520942616725 | 0.1754042948362080 |
| 0.3448646700244386 | 0.0660418626521450 | 0.0445925961358658 |
| 0.1254714896780223 | 0.2038894814514353 | 0.4525949150838544 |
| 0.1640263202888573 | 0.2370112324975344 | 0.1576936426462709 |
| 0.3815944982851869 | 0.1839334948814777 | 0.1542610115119534 |
| 0.2752981387437006 | 0.1319686381771642 | 0.1991950273421710 |
| 0.2178400378083776 | 0.1006641296047462 | 0.3314321676072389 |
| 0.2212372382454060 | 0.1584907556288503 | 0.4074686768477471 |
| 0.1490704832920845 | 0.0122246206123163 | 0.3919159049976113 |
| 0.3107391703306801 | 0.0306100527132174 | 0.1434650431498813 |

Type A isomerisation, configuration R5 of the reactant

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1209577156767000 | 0.7362052039669277 | 0.2772029613118491 |
| 0.6214522325416657 | 0.2255547196663348 | 0.7780622249594401 |
| 0.8511769355359545 | 0.4592870394891289 | 0.3156860883087116 |

| | | |
|--------------------|--------------------|--------------------|
| 0.3434283054148127 | 0.9639712465733069 | 0.8223263518367643 |
| 0.8874611151962716 | 0.1905876374729232 | 0.0447747999638268 |
| 0.4037884266669539 | 0.6813385834103840 | 0.5532083624903706 |
| 0.7462548899193555 | 0.3575800749864611 | 0.2083758925771832 |
| 0.2429714766523233 | 0.8508619891291027 | 0.7132762141509340 |
| 0.0176514262690287 | 0.6262666872587888 | 0.1737642227613434 |
| 0.5132413841832545 | 0.1289485567161663 | 0.6677568919551711 |
| 0.2907758888979469 | 0.5822215011603966 | 0.4440114979885975 |
| 0.7853628023442322 | 0.0820135890138062 | 0.9440409098238485 |
| 0.2818864908738504 | 0.3619052199065009 | 0.6750977159742277 |
| 0.7876062633272265 | 0.8570234380109986 | 0.1703033536199663 |
| 0.7323971532131187 | 0.1363619994442387 | 0.4359862506962241 |
| 0.2452309960082668 | 0.6255136800673549 | 0.9428777600391505 |
| 0.3928503774281503 | 0.4583691037128870 | 0.7815984525635910 |
| 0.8924461911407059 | 0.9666663421236974 | 0.2739881334973090 |
| 0.1206752295204890 | 0.1905105819426162 | 0.8127815433146520 |
| 0.6191976707926490 | 0.6933849168954187 | 0.3162574262806764 |
| 0.3475349057877495 | 0.7383691273874149 | 0.0465858321262178 |
| 0.8431565368513073 | 0.2393774072331041 | 0.5464825597227321 |
| 0.5138614936825365 | 0.5893019017176302 | 0.2142285962328934 |
| 0.0203179373977719 | 0.0835696613526405 | 0.7033492773898949 |
| 0.2276084016012630 | 0.7763888993440725 | 0.1557297954035610 |
| 0.7287736367225363 | 0.2722955866627325 | 0.6633491708768040 |
| 0.2276295392679453 | 0.0738141158180941 | 0.8639196112462477 |
| 0.7315770648816909 | 0.5730680639093592 | 0.3349053527634803 |
| 0.9324265892682723 | 0.0762531395455193 | 0.1558187487049023 |
| 0.4410401749872797 | 0.5646176080953456 | 0.6650875805468932 |
| 0.6951219068052686 | 0.2494640926308322 | 0.3206031483580674 |
| 0.2092573236204906 | 0.7344820060953164 | 0.8279500625038981 |
| 0.4050580746634238 | 0.2541885651876701 | 0.6400205554608881 |
| 0.9067314055798888 | 0.7449089770233623 | 0.1388283733620847 |
| 0.4085118693770802 | 0.5402660347731507 | 0.3334379939353753 |
| 0.9046349166680324 | 0.0557291225433337 | 0.8370048141786006 |
| 0.1740965894586697 | 0.6651647039157587 | 0.3931925171323966 |
| 0.6614331174737503 | 0.1532484162555596 | 0.9017573040227733 |
| 0.4611705628227116 | 0.0130693399023422 | 0.7384171454323533 |
| 0.9709419285406692 | 0.5064811025739512 | 0.2448860058560579 |
| 0.8166983704378912 | 0.3138569006024642 | 0.0871148714889558 |
| 0.3341073138666379 | 0.8022456555861316 | 0.5958300623513636 |
| 0.4644280997710266 | 0.6573552123974034 | 0.0967615313891930 |
| 0.9670385182546043 | 0.1601022735492297 | 0.5776681781480297 |
| 0.1661119504669295 | 0.3118273379291364 | 0.7544682444480182 |
| 0.6663613578885783 | 0.8126187771075705 | 0.2483316226967669 |
| 0.8152365953003485 | 0.0152687378127029 | 0.3924076686595799 |
| 0.3250787917408804 | 0.5003513531383716 | 0.9050840212624639 |
| 0.0123980158996129 | 0.8573292586090175 | 0.3009508533317333 |
| 0.5066589583053684 | 0.3412893820187451 | 0.8067606121562154 |
| 0.8607967041301039 | 0.3680939275176631 | 0.4469939751958900 |
| 0.3754455834616686 | 0.8601545253673496 | 0.9436754422767825 |
| 0.0037799501628571 | 0.2118279631150372 | 0.9302936570657663 |
| 0.5264411702384325 | 0.7043485063585425 | 0.4474650126046157 |
| 0.6294805512191513 | 0.4742388500770644 | 0.1866695585744558 |
| 0.1249991582834507 | 0.9483335507364422 | 0.6805890460478556 |
| 0.1237797733630370 | 0.6021783133828005 | 0.0515659360569434 |
| 0.6081138110556294 | 0.1106959629111612 | 0.5378378786605617 |
| 0.2602642984783997 | 0.4607809212091540 | 0.5473301925802284 |
| 0.7613283795488567 | 0.9566026213235518 | 0.0471629460074109 |
| 0.0715519881039095 | 0.6454875970074737 | 0.2596650444580354 |

| | | |
|--------------------|--------------------|--------------------|
| 0.5797170795577461 | 0.1368641447329646 | 0.7489354268078531 |
| 0.8405820833731843 | 0.3921916716212462 | 0.2362274752462956 |
| 0.3195412877876977 | 0.9044369442933055 | 0.7461496331378288 |
| 0.7891818506525077 | 0.1646651344876691 | 0.0138363136286165 |
| 0.3204367756206559 | 0.6582335815692399 | 0.4996080338298453 |
| 0.0927165794688201 | 0.1703626320023765 | 0.7118124575888111 |
| 0.5508514918728620 | 0.6858229763888829 | 0.2361709330131584 |
| 0.2973425547903659 | 0.4253267517098888 | 0.7543179759551759 |
| 0.8064256946023443 | 0.9164293619010530 | 0.2511102150840536 |
| 0.3271482212138384 | 0.6542146901218066 | 0.9926933204953503 |
| 0.8062000916100847 | 0.1701129344631958 | 0.4887391368233559 |
| 0.5221720018063435 | 0.3403676460960390 | 0.1337371545187264 |
| 0.4226425969571327 | 0.1033152865333437 | 0.4704957922736201 |
| 0.3649785607628445 | 0.2654289745149885 | 0.4429680462116104 |
| 0.2638615228926960 | 0.1738432084400888 | 0.5323171747084329 |
| 0.1153818264080611 | 0.2814029177379341 | 0.4142364342924675 |
| 0.2009030957463233 | 0.3868950595336500 | 0.3354927167577286 |
| 0.1693379557786080 | 0.3242096165695513 | 0.2528217493825123 |
| 0.3793709852676043 | 0.3730581751734203 | 0.1124020468998156 |
| 0.6083167581432505 | 0.1311599831894810 | 0.2051463820163225 |
| 0.5292069630869866 | 0.1158537384113125 | 0.1306958977484502 |
| 0.5188305126784084 | 0.0241391375327139 | 0.2839291650658261 |
| 0.1975205997814251 | 0.0722327385875949 | 0.4451247353301893 |
| 0.3536452970148837 | 0.9964855623502920 | 0.3952720045341960 |
| 0.2670283054728533 | 0.0772083218297981 | 0.2892185915864713 |
| 0.3795588509105550 | 0.4008358211600354 | 0.2371560906436446 |
| 0.3455685671534842 | 0.1838522957746222 | 0.4543974434983378 |
| 0.1917110195911526 | 0.3042510464047515 | 0.3355828262948592 |
| 0.3054754839238930 | 0.1961559661342232 | 0.3441657337944244 |
| 0.4175236050530521 | 0.2151248124445759 | 0.2507068649287559 |
| 0.4281684107725564 | 0.3381089971584059 | 0.1812768072192336 |
| 0.5235306759246949 | 0.1140270407558727 | 0.2217002073462678 |
| 0.2808113226707507 | 0.0777608743436157 | 0.3693017236024891 |

Type A isomerization, configuration TS5 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

Si Al O H C

23 1 48 15 7

direct

| | | |
|----------------|----------------|----------------|
| 0.119287624021 | 0.740917600955 | 0.273432281860 |
| 0.623875458024 | 0.232965827373 | 0.767529218935 |
| 0.852954540323 | 0.463244581932 | 0.308885003023 |
| 0.344780376404 | 0.968726670525 | 0.821529920290 |
| 0.887059765124 | 0.191885545339 | 0.041416389894 |
| 0.403019243710 | 0.685790901282 | 0.549509631085 |
| 0.745423273975 | 0.363850720749 | 0.201439786565 |
| 0.244359095903 | 0.854255780777 | 0.711801261790 |
| 0.018961058934 | 0.629841089824 | 0.168390743413 |
| 0.510895004400 | 0.134489423278 | 0.662151337572 |
| 0.288284887846 | 0.589289814589 | 0.443386171729 |
| 0.790253926169 | 0.081556559319 | 0.940176670924 |
| 0.281052301933 | 0.365104886980 | 0.671837062810 |
| 0.789846894574 | 0.857063791053 | 0.162174953857 |
| 0.736584062100 | 0.134232060414 | 0.434878839914 |
| 0.248381662460 | 0.629692699895 | 0.938665344717 |

| | | |
|----------------|----------------|----------------|
| 0.397557401475 | 0.460859630280 | 0.776650745392 |
| 0.892363807471 | 0.967862152583 | 0.268865899066 |
| 0.122841691496 | 0.194084929442 | 0.810791159149 |
| 0.626160861375 | 0.689242543176 | 0.315456054856 |
| 0.347483126720 | 0.743335269273 | 0.043762486032 |
| 0.845083063901 | 0.235270727760 | 0.541326135080 |
| 0.515366627168 | 0.586930462331 | 0.212954823499 |
| 0.024407950810 | 0.083060372225 | 0.705812307063 |
| 0.223772946024 | 0.781216924676 | 0.149716156469 |
| 0.722429523263 | 0.284588936958 | 0.644079259676 |
| 0.231715976718 | 0.080830830167 | 0.862365415155 |
| 0.736505824558 | 0.571795371242 | 0.351784897614 |
| 0.932761445530 | 0.078267675038 | 0.152504125906 |
| 0.444280277379 | 0.565659160425 | 0.656654116174 |
| 0.708840602765 | 0.254805019595 | 0.322213261401 |
| 0.206729791793 | 0.740298382817 | 0.826611217127 |
| 0.399076344332 | 0.255084408542 | 0.631498268257 |
| 0.909245014109 | 0.746214802363 | 0.126805508609 |
| 0.410047510395 | 0.546690981350 | 0.337001831845 |
| 0.918764233981 | 0.047133036103 | 0.845160441922 |
| 0.174625445409 | 0.669155307545 | 0.387810036955 |
| 0.677647385174 | 0.154409182221 | 0.881468010340 |
| 0.463575740118 | 0.015368074367 | 0.733557487996 |
| 0.973724792474 | 0.508927499910 | 0.240601934238 |
| 0.818649217887 | 0.314801170894 | 0.083916402108 |
| 0.340969569748 | 0.804359043266 | 0.596280862261 |
| 0.460475355218 | 0.664167338434 | 0.099619043700 |
| 0.960876416332 | 0.164323798714 | 0.587908998266 |
| 0.163035916902 | 0.318576405822 | 0.753313344948 |
| 0.671445485689 | 0.809220022390 | 0.243815541395 |
| 0.807846501506 | 0.015184455791 | 0.387155225464 |
| 0.327087691401 | 0.507436186138 | 0.896649244060 |
| 0.012633747561 | 0.862179013107 | 0.299735217007 |
| 0.512908771006 | 0.347214516357 | 0.805214399267 |
| 0.873632877739 | 0.351773195724 | 0.426903486835 |
| 0.377278166410 | 0.865513854285 | 0.942704516836 |
| 0.003367021485 | 0.212769327433 | 0.926395453219 |
| 0.521493437713 | 0.710726376249 | 0.438252574077 |
| 0.618854781005 | 0.465794053729 | 0.182621206145 |
| 0.130391060546 | 0.952771357421 | 0.670852626163 |
| 0.129828342067 | 0.603249677890 | 0.050074017813 |
| 0.606650346307 | 0.117971359439 | 0.531734691193 |
| 0.256847634127 | 0.468128179122 | 0.546790526046 |
| 0.757194086237 | 0.959353713056 | 0.042704668602 |
| 0.065468742496 | 0.652828529296 | 0.257705794445 |
| 0.572856700922 | 0.148191042295 | 0.743251644577 |
| 0.829959131287 | 0.421879281570 | 0.216125771097 |
| 0.316388665758 | 0.909844759413 | 0.748042735067 |
| 0.788138896607 | 0.166089257012 | 0.011510514762 |
| 0.311145829043 | 0.668655672880 | 0.501244151767 |
| 0.101305053456 | 0.169696653760 | 0.708008352982 |
| 0.572979232722 | 0.670305557745 | 0.229643735841 |
| 0.305930145688 | 0.420629731050 | 0.751286186764 |
| 0.812667517139 | 0.913900801219 | 0.242239954177 |
| 0.332197565693 | 0.660363797885 | 0.984550634266 |
| 0.817619023484 | 0.147478751843 | 0.496375027064 |
| 0.535191634944 | 0.257096560954 | 0.286107754588 |
| 0.382799658051 | 0.007537611854 | 0.487303640148 |

| | | |
|----------------|----------------|----------------|
| 0.422473046916 | 0.131579969504 | 0.485636259034 |
| 0.269939568029 | 0.131051874797 | 0.548679820017 |
| 0.098424339192 | 0.277851734317 | 0.463693025725 |
| 0.210172117385 | 0.351144051322 | 0.420405126983 |
| 0.152710579369 | 0.358611955964 | 0.309676670301 |
| 0.438979085573 | 0.342976198946 | 0.191156267003 |
| 0.578801407248 | 0.059942476186 | 0.273712692976 |
| 0.509851880771 | 0.126694941718 | 0.155799192448 |
| 0.467044322574 | 0.003826073925 | 0.281082920236 |
| 0.149148057856 | 0.081405267999 | 0.444556258384 |
| 0.291505088401 | 0.013288984459 | 0.350883092215 |
| 0.186827192565 | 0.145014843745 | 0.284252582044 |
| 0.385238436017 | 0.345182546042 | 0.344423020149 |
| 0.354669869960 | 0.104061707670 | 0.478274670859 |
| 0.179294223987 | 0.300059888067 | 0.392808118813 |
| 0.274446453723 | 0.186219703916 | 0.366382076844 |
| 0.398847058068 | 0.181051166539 | 0.313728489917 |
| 0.441133768323 | 0.287447795071 | 0.284534219702 |
| 0.492765008990 | 0.085742010313 | 0.254731507494 |
| 0.224048360772 | 0.099507146144 | 0.362102256982 |

Type A isomerisation, configuration P5 of the product

1.000000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1215235715885762 | 0.7369017644612506 | 0.2718889971995356 |
| 0.6216613000110705 | 0.2352387920370835 | 0.7694597304729796 |
| 0.8530827047759573 | 0.4636110185764807 | 0.3110183220501901 |
| 0.3492733509827088 | 0.9653531672798611 | 0.8195509992693567 |
| 0.8924628454424089 | 0.1900701075838416 | 0.0433864836617061 |
| 0.4007603475122898 | 0.6845503594741938 | 0.5483151387052422 |
| 0.7450312471870328 | 0.3579764577420768 | 0.2065139754594922 |
| 0.2472951629087958 | 0.8577928643955618 | 0.7049761505134462 |
| 0.0158922630258525 | 0.6324745773285062 | 0.1647175084978603 |
| 0.5146122191439237 | 0.1303959290921283 | 0.6669434575321954 |
| 0.2894094814267770 | 0.5860494408388781 | 0.4431609058343713 |
| 0.7951207823919275 | 0.0797589803214040 | 0.9397736634975646 |
| 0.2878780489531892 | 0.3596520650186590 | 0.6683041083028706 |
| 0.7842981369946862 | 0.8607915771221907 | 0.1664810321905720 |
| 0.7431640808765336 | 0.1327986580813482 | 0.4350756399762157 |
| 0.2428944491261747 | 0.6339218712432493 | 0.9336447343842024 |
| 0.3991614201076896 | 0.4614110999010915 | 0.7755996156627528 |
| 0.8934921980053027 | 0.9649956631876164 | 0.2719779084955142 |
| 0.1261947072247070 | 0.1922342584630115 | 0.8140772526122797 |
| 0.6240865411978261 | 0.6915243340712270 | 0.3101719124102484 |
| 0.3477908334580767 | 0.7395128993114094 | 0.0424951982656867 |
| 0.8430123524112042 | 0.2418292513354943 | 0.5414447088670965 |
| 0.5177099921550898 | 0.5867562897399312 | 0.2097105572811109 |
| 0.0233038371978139 | 0.0822194546376615 | 0.7103711634526996 |
| 0.2267815647775477 | 0.7792203892807347 | 0.1501684549996481 |
| 0.7120831788317911 | 0.2865379388490600 | 0.6377422141462564 |
| 0.2369875055523421 | 0.0775888439991626 | 0.8606398024725472 |
| 0.7364105832204351 | 0.5756479645098873 | 0.3447585768305605 |
| 0.9342266418012870 | 0.0749558024164544 | 0.1554932213779783 |

0.4445578092662158 0.5678469295123533 0.6567828361144297
0.7029785295686307 0.2481191336195352 0.3232233659568073
0.2056873645415775 0.7458070268993909 0.8199443113179000
0.4040883593486921 0.2484910324787152 0.6278906709615685
0.9027563545920906 0.7487793925455828 0.1315372579459348
0.4137202750758269 0.5502515670124389 0.3364930146373744
0.9245783158959230 0.0325991212610214 0.8508013612922933
0.1757079164239320 0.6623611222214486 0.3870645957356709
0.6879067584567771 0.1575419993869049 0.8741279396171949
0.4697548856252455 0.0097748792994804 0.7349268921975782
0.9741522843813754 0.5091221560411257 0.2363961109656685
0.8209425645152313 0.3120812953909730 0.0872444677371383
0.3415493035403464 0.8061595748645676 0.5900817890576893
0.4614591325652431 0.6561462552794546 0.0968762046329397
0.9511946998162434 0.1693436102238838 0.5993025170649474
0.1690035220177848 0.3154542794502200 0.7524997343825944
0.6651050573230092 0.8139796393727869 0.2465656886945016
0.8152501276731221 0.0110830096952491 0.3917243156544634
0.3195500948318767 0.5104699949144874 0.8935105275582934
0.0137166898122586 0.8567175474563614 0.2997689824883284
0.5150380271181609 0.3511658384470735 0.8096514485886630
0.8759482951684401 0.3618603367960606 0.4346852268830148
0.3796981517732945 0.8603393329108036 0.9408023256222284
0.0123419682860840 0.2116767161559395 0.9339219337283504
0.5173666293487623 0.7052886786407500 0.4335325938330424
0.6220009159228610 0.4642204578779838 0.1845606649335363
0.1354878427127660 0.9603526494187954 0.6608204217486042
0.1208376821697252 0.6115560005752392 0.0413497218458646
0.6214522422306562 0.1110811746759475 0.5433605833408672
0.2625261407646583 0.4612885173442389 0.5428626158924961
0.7522303609206850 0.9644606499153501 0.0472336180393461
0.0696852217666801 0.6498118634993433 0.2519389823463359
0.5621080091680458 0.1500037838656123 0.7568181641113176
0.8309218107475248 0.4079624536123507 0.2295546800092759
0.3207448012574911 0.9097873140970377 0.7430231433744673
0.7980915043174259 0.1665176545761863 0.0051963246944253
0.3046690192783436 0.6649052846945870 0.5075116855953747
0.0946420340164233 0.1707428730237390 0.7164012719856160
0.5759398453356029 0.6749536404647354 0.2185038293182928
0.3161459330595616 0.4152740925608118 0.7448916538119579
0.8086652413445733 0.9151103655654289 0.2476572369557225
0.3259937715202594 0.6602157028257463 0.9841722817398012
0.8311096756006568 0.1584450070410312 0.4789170786199197
0.5210764038657012 0.2663013509593617 0.2624364499159791
0.3957622920396467 0.0045786040470589 0.4758885941596043
0.5068144593321796 0.0791847391676455 0.4344938043502883
0.3573686851933142 0.1327486168201345 0.5269653917675404
0.0856099998200664 0.2824628192867408 0.4901179684937393
0.2103650452464416 0.3440679330394726 0.4459792466915503
0.1341063646660185 0.3732508293406095 0.3416603610915857
0.3909104014374205 0.3623516132531023 0.2122099803864970
0.5490960092487087 0.0984877709374087 0.2108068477467019
0.4262900091010385 0.1660282610154916 0.1474631991496757
0.4388304671174822 0.0227148777602324 0.2628096270908417
0.1840752719115648 0.0531729431750423 0.4732646666990787
0.2497121028745621 0.0616255951019632 0.3150126052080553
0.1010178595790003 0.1606782566653154 0.3748968209881524
0.3893587242203692 0.3333821575157284 0.3637039634643645

| | | |
|--------------------|--------------------|--------------------|
| 0.4102497241938863 | 0.0922904800318161 | 0.4519505690593643 |
| 0.1674493114404370 | 0.3033134230059643 | 0.4194058096592460 |
| 0.2494043544034288 | 0.2010706266421385 | 0.3718763398925827 |
| 0.3816502435949648 | 0.1802772925426158 | 0.3282265990681970 |
| 0.4216352204249021 | 0.2930976026646060 | 0.2899844251720030 |
| 0.4518474837149155 | 0.1124337578020988 | 0.2317888181163278 |
| 0.1952394022052906 | 0.1161678675767690 | 0.3780981127329849 |

Type A isomerisation, configuration R6 of the reactant

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1120105965250757 | 0.7449900714851994 | 0.2777381210614993 |
| 0.6139985336138452 | 0.2343088230798884 | 0.7755476491919556 |
| 0.8471027070448144 | 0.4648522523707722 | 0.3130079458463638 |
| 0.3345691802262344 | 0.9734734025759360 | 0.8247053768131786 |
| 0.8787284636976621 | 0.1990450775853216 | 0.0438078991902113 |
| 0.3971707580360747 | 0.6876212696321435 | 0.5556829582224712 |
| 0.7375789607626040 | 0.3662295197833382 | 0.2075501907829000 |
| 0.2369384587009867 | 0.8573907981669171 | 0.7144185909353361 |
| 0.0099276889660321 | 0.6337493399344918 | 0.1754155076537828 |
| 0.5034556350254482 | 0.1380118449926632 | 0.6652641753198211 |
| 0.2828743715709397 | 0.5942157230877715 | 0.4455995828590837 |
| 0.7800850917537870 | 0.0845105993528452 | 0.9431741215099426 |
| 0.2728956310155446 | 0.3694347525670284 | 0.6749613634074929 |
| 0.7807016635360411 | 0.8627216975947001 | 0.1716223167471147 |
| 0.7236331712185988 | 0.1444357842784132 | 0.4358480804980706 |
| 0.2399711239158979 | 0.6332435826848083 | 0.9429805835179302 |
| 0.3841622963635378 | 0.4626388983977017 | 0.7849843654656703 |
| 0.8860751732662896 | 0.9750818341781401 | 0.2734604717945684 |
| 0.1113625547058065 | 0.1987269647562299 | 0.8138747049912511 |
| 0.6143354630771892 | 0.6988755305644929 | 0.3179050063029038 |
| 0.3403240533591088 | 0.7467173100811070 | 0.0460304612359530 |
| 0.8342892019781371 | 0.2467369621787356 | 0.5467161773936070 |
| 0.5067891286933266 | 0.5991254867822453 | 0.2157114329037408 |
| 0.0130488667380298 | 0.0854238377357372 | 0.7054541069460221 |
| 0.2168734706676335 | 0.7822011130740804 | 0.1531197807971196 |
| 0.7174116667121464 | 0.2860171854356979 | 0.6594102768933883 |
| 0.2202813728700816 | 0.0850023752331199 | 0.8650527412198645 |
| 0.7287135312028891 | 0.5797543468827500 | 0.3326220765203007 |
| 0.9235779655580555 | 0.0856351698329266 | 0.1554115398526241 |
| 0.4309307539518638 | 0.5683297477859273 | 0.6670610247812853 |
| 0.6867254125833213 | 0.2589492048087783 | 0.3214539563056429 |
| 0.2021029472089779 | 0.7406808805118361 | 0.8280199724523128 |
| 0.3945784472847995 | 0.2620273908134447 | 0.6358330437671557 |
| 0.8976705288672854 | 0.7497068657188177 | 0.1381883122772532 |
| 0.4034595886981948 | 0.5515808495074467 | 0.3379890549738582 |
| 0.9012422070097537 | 0.0499064773028018 | 0.8409882287060894 |
| 0.1680560673622735 | 0.6746294965534654 | 0.3916090637355887 |
| 0.6592892963340174 | 0.1569443647591965 | 0.8957540323840462 |
| 0.4528715877841649 | 0.0212432771520683 | 0.7386042959634377 |
| 0.9678319627820088 | 0.5109484126144248 | 0.2430625420385968 |
| 0.8042467348353465 | 0.3217169577383957 | 0.0867969653938087 |
| 0.3346274213108237 | 0.8081524460387161 | 0.5988677773146932 |

| | | |
|--------------------|--------------------|--------------------|
| 0.4545665361152441 | 0.6673198970633395 | 0.1002090916713498 |
| 0.9544563738943421 | 0.1653930794243319 | 0.5837489409853697 |
| 0.1556573849309819 | 0.3211832937899692 | 0.7500163258767688 |
| 0.6588351215272028 | 0.8199340593039718 | 0.2546009695850194 |
| 0.8059884460617868 | 0.0238249917333042 | 0.3914749275317250 |
| 0.3153568726164016 | 0.5064780863868680 | 0.9073440264013168 |
| 0.0070920876099600 | 0.8683222641044547 | 0.3011864418023173 |
| 0.4989258771195344 | 0.3470026495559293 | 0.8120389801570826 |
| 0.8573467469039600 | 0.3720691668258367 | 0.4436305062316185 |
| 0.3672344549702277 | 0.8704893346353434 | 0.9462700102082905 |
| 0.9960800827982809 | 0.2225558020345350 | 0.9318552934798537 |
| 0.5221056605372587 | 0.7037692482404125 | 0.4506026074597382 |
| 0.6211985569257330 | 0.4835766011125720 | 0.1875598856287324 |
| 0.1206204603963752 | 0.9533133579520722 | 0.6769976196634365 |
| 0.1199701793350711 | 0.6120881784090536 | 0.0548988340191792 |
| 0.5982411318453266 | 0.1185499837898552 | 0.5354949568130680 |
| 0.2511341586941289 | 0.4738514461683166 | 0.5499147485728844 |
| 0.7495901553082143 | 0.9635729095862755 | 0.0508792849041782 |
| 0.0564662098832020 | 0.6560043530839950 | 0.2652993946435293 |
| 0.5700202626142410 | 0.1488290530829621 | 0.7444899558153293 |
| 0.8347130252641068 | 0.3996752786353889 | 0.2328038666133434 |
| 0.3077700213589760 | 0.9129815661704712 | 0.7518795537088503 |
| 0.7848432918068716 | 0.1704545404956744 | 0.0089534878179264 |
| 0.3083379589123482 | 0.6728097234966867 | 0.5019685301356357 |
| 0.0806255982650667 | 0.1737769000221626 | 0.7181020113982235 |
| 0.5472481746818885 | 0.6954254127548885 | 0.2342719606363302 |
| 0.2905956675823498 | 0.4247542739536506 | 0.7599475929048757 |
| 0.8039722247613283 | 0.9209275970386934 | 0.2500857780535942 |
| 0.3261401134063682 | 0.6629204148913999 | 0.9867923104021707 |
| 0.7968248227975561 | 0.1758184758764445 | 0.4911185180720656 |
| 0.3428898024802751 | 0.3234885798490481 | 0.0984311185731362 |
| 0.2500586766408004 | 0.3676426618183871 | 0.4142462590452547 |
| 0.4112112725823379 | 0.3238997558144193 | 0.3511875327422761 |
| 0.3151248516005499 | 0.4091906986995114 | 0.2528892342231271 |
| 0.1679705251491921 | 0.3195623112794732 | 0.2542251713145778 |
| 0.1749501215780793 | 0.1632979194072585 | 0.3313933390388169 |
| 0.1142175974538431 | 0.2683099807340810 | 0.4152088194566259 |
| 0.4792388894612259 | 0.2082276163274825 | 0.0512481329153652 |
| 0.5483083409167462 | 0.0314009048413418 | 0.2610468585067912 |
| 0.5471668656053663 | 0.1242045177908714 | 0.3352044635743375 |
| 0.6043543023776727 | 0.1568211888408827 | 0.1700208766503961 |
| 0.4049132184352512 | 0.1137110995221645 | 0.4876638619924383 |
| 0.3229571391079171 | 0.0354959581245911 | 0.4753382238364165 |
| 0.2438656637408456 | 0.1568948935175217 | 0.5417442903890602 |
| 0.3326288619975767 | 0.1799602312058860 | 0.1326033892314294 |
| 0.3250962921995889 | 0.3385273706309130 | 0.3383575256055589 |
| 0.1847250313523958 | 0.2441546097527724 | 0.3349442039391948 |
| 0.3094916250685532 | 0.2163304615412342 | 0.3471292778260919 |
| 0.4122272883460741 | 0.1898585241040859 | 0.2425633374310421 |
| 0.3946451770237886 | 0.2264322585910706 | 0.1235795577608404 |
| 0.5347750552347023 | 0.1269999613785231 | 0.2533543040843214 |
| 0.3225362559663592 | 0.1245477696465696 | 0.4700490107557201 |

Type A isomerization, configuration TS6 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

Si Al O H C
23 1 48 15 7
direct

| | | |
|----------------|----------------|----------------|
| 0.107280768209 | 0.741732138489 | 0.278157369369 |
| 0.615683361779 | 0.238763292735 | 0.769735622788 |
| 0.843453995265 | 0.466504880191 | 0.312011328696 |
| 0.334521569451 | 0.973188034561 | 0.826726810808 |
| 0.878025480200 | 0.195555807805 | 0.044472910461 |
| 0.393590965034 | 0.689548463689 | 0.551926454448 |
| 0.730289907933 | 0.365204420908 | 0.206979686340 |
| 0.238074669975 | 0.858686963987 | 0.714211689763 |
| 0.009080227999 | 0.632146902861 | 0.171189072037 |
| 0.500252720583 | 0.138417842979 | 0.665651147295 |
| 0.277742178049 | 0.595535879835 | 0.448056007941 |
| 0.784164264236 | 0.083476080617 | 0.939814407756 |
| 0.272474135374 | 0.367708368595 | 0.675808876444 |
| 0.780167207569 | 0.861160179010 | 0.165191473597 |
| 0.723728920348 | 0.138750668439 | 0.436805426882 |
| 0.239418599106 | 0.635601073681 | 0.939985514710 |
| 0.390353358036 | 0.463549518027 | 0.779580564870 |
| 0.882199548646 | 0.971034108827 | 0.272566322337 |
| 0.111037853488 | 0.200241221285 | 0.813646533552 |
| 0.617850737593 | 0.693813435302 | 0.316214118658 |
| 0.335858014505 | 0.747762772796 | 0.047522629988 |
| 0.836093852448 | 0.241454209620 | 0.542334409959 |
| 0.505445337794 | 0.591962901420 | 0.216108275103 |
| 0.016588336684 | 0.087303822422 | 0.704955321114 |
| 0.210381017180 | 0.781680150897 | 0.153079914587 |
| 0.714431273446 | 0.289964268081 | 0.646673514916 |
| 0.220248228491 | 0.086102123077 | 0.863528550182 |
| 0.730400802793 | 0.578898778572 | 0.351550979583 |
| 0.922559957785 | 0.081253081600 | 0.155770945130 |
| 0.435246048252 | 0.566510586936 | 0.656711221474 |
| 0.687562294164 | 0.255951495518 | 0.324114658587 |
| 0.196099586785 | 0.746415015452 | 0.829326173096 |
| 0.388065412169 | 0.257588532254 | 0.631285848616 |
| 0.899236342385 | 0.749358838036 | 0.131237701343 |
| 0.401515091733 | 0.553982489389 | 0.342640204387 |
| 0.911844280419 | 0.047338690065 | 0.844874903665 |
| 0.164680266560 | 0.670592852618 | 0.391169945234 |
| 0.670337525853 | 0.156173727849 | 0.882675626984 |
| 0.454211931552 | 0.019079399027 | 0.742382303081 |
| 0.965389868694 | 0.510262059130 | 0.236399730958 |
| 0.805743327805 | 0.317596125045 | 0.088660612802 |
| 0.336620652434 | 0.805428448699 | 0.601573223066 |
| 0.447751619544 | 0.669126369916 | 0.104949861720 |
| 0.951239026270 | 0.163340864751 | 0.588437434890 |
| 0.152973728979 | 0.323877390607 | 0.755881548080 |
| 0.659987458196 | 0.815792342227 | 0.245713270788 |
| 0.799185542939 | 0.018790482160 | 0.390790453891 |
| 0.317359306921 | 0.513448015767 | 0.897466731325 |
| 0.001396368232 | 0.863499870320 | 0.303889872488 |
| 0.507086536686 | 0.353179397882 | 0.811010630846 |
| 0.866795667309 | 0.359937987955 | 0.432088877079 |
| 0.363691201784 | 0.872010239042 | 0.950324152619 |
| 0.994774623442 | 0.219425746866 | 0.931853700484 |
| 0.511673672303 | 0.711542357994 | 0.438995416035 |
| 0.604905145642 | 0.468795794316 | 0.185696283705 |

| | | |
|----------------|----------------|----------------|
| 0.126544649347 | 0.958647414803 | 0.670598605653 |
| 0.122261317452 | 0.608377544024 | 0.053253635238 |
| 0.597581650079 | 0.116936197543 | 0.537805370858 |
| 0.248976896106 | 0.473703264161 | 0.552117531903 |
| 0.749931704484 | 0.962761507471 | 0.044478737695 |
| 0.053484505583 | 0.651963977626 | 0.264568509765 |
| 0.559878692049 | 0.159210840972 | 0.744066010627 |
| 0.813421550095 | 0.419430558694 | 0.228422705067 |
| 0.310394851730 | 0.911019667193 | 0.753469007149 |
| 0.782754585563 | 0.169652368102 | 0.009279605431 |
| 0.296774106426 | 0.677590811589 | 0.505698958427 |
| 0.084429750972 | 0.179109493622 | 0.712400508416 |
| 0.569118857398 | 0.672739859217 | 0.228047114659 |
| 0.301787730147 | 0.416063949747 | 0.758033078156 |
| 0.801781660673 | 0.918072253017 | 0.245887183980 |
| 0.325439913062 | 0.664865618064 | 0.984579385450 |
| 0.803512811301 | 0.162701906620 | 0.490998663074 |
| 0.281480325502 | 0.365293309466 | 0.154135824483 |
| 0.365043423855 | 0.306266629409 | 0.436573786550 |
| 0.476691447331 | 0.316384455690 | 0.296539588091 |
| 0.321198748624 | 0.409083863304 | 0.300295815830 |
| 0.156754914107 | 0.343608120169 | 0.316880076332 |
| 0.141378696389 | 0.196411086717 | 0.408823650205 |
| 0.140758377046 | 0.293357433771 | 0.475957386271 |
| 0.440697277471 | 0.342737680022 | 0.078067564527 |
| 0.524133288612 | 0.056454132059 | 0.215465256507 |
| 0.559808697123 | 0.088653938532 | 0.318142892750 |
| 0.593071415762 | 0.173142288821 | 0.160484187302 |
| 0.438698775761 | 0.081323301880 | 0.483870853594 |
| 0.337591100316 | 0.021948182511 | 0.476489220227 |
| 0.280885309464 | 0.122546087667 | 0.564841271496 |
| 0.371276313123 | 0.238104114200 | 0.097563929135 |
| 0.380025623326 | 0.322435873829 | 0.339933602219 |
| 0.181836695224 | 0.265938345697 | 0.392460277739 |
| 0.316327798543 | 0.207495360246 | 0.373210723434 |
| 0.402597085123 | 0.217567246124 | 0.256612072732 |
| 0.370626111662 | 0.297749808182 | 0.141504393013 |
| 0.527583152900 | 0.130254853675 | 0.237938836645 |
| 0.346640687932 | 0.102805208832 | 0.480782597182 |

Type A isomerisation, configuration P6 of the product

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C |
|----|----|----|----|---|
| 23 | 1 | 48 | 15 | 7 |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1168395357950788 | 0.7387376796707467 | 0.2759655621043948 |
| 0.6176356524677438 | 0.2339363390469364 | 0.7780095162140910 |
| 0.8480028350771412 | 0.4643913993784861 | 0.3108045970826559 |
| 0.3424903784936545 | 0.9677355233341893 | 0.8237488321530726 |
| 0.8870184625503628 | 0.1932824969662773 | 0.0447014845836037 |
| 0.3971336530042157 | 0.6873317999442524 | 0.5517144674304596 |
| 0.7413813820594950 | 0.3602839879316175 | 0.2091495644477155 |
| 0.2426561496628290 | 0.8580726060767225 | 0.7092284762024188 |
| 0.0116023287385617 | 0.6326607130107813 | 0.1715110955279121 |
| 0.5105413784788952 | 0.1329437611405540 | 0.6675625955453965 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2852740320544023 | 0.5896376217154941 | 0.4448866373411316 |
| 0.7830830926743190 | 0.0826080534165230 | 0.9404741165304213 |
| 0.2802911225775254 | 0.3634529832706441 | 0.6722300948435329 |
| 0.7790222643370123 | 0.8636482790717194 | 0.1737989399305145 |
| 0.7322058895309377 | 0.1380913024866662 | 0.4388971845519062 |
| 0.2380431416775117 | 0.6333073230596982 | 0.9391276127821199 |
| 0.3878900230733151 | 0.4626782444463213 | 0.7812718005127555 |
| 0.8876856452224640 | 0.9695645029193493 | 0.2756170220353549 |
| 0.1170382244145293 | 0.1938095257586513 | 0.8188954019534936 |
| 0.6151672065505999 | 0.6980824002308909 | 0.3119050179780522 |
| 0.3427930980395625 | 0.7409285425876144 | 0.0461752844172692 |
| 0.8397311186332703 | 0.2459528395185996 | 0.5462547678111913 |
| 0.5104800063175894 | 0.5937561193999733 | 0.2130870073827598 |
| 0.0143194921879509 | 0.0840484486807589 | 0.7060397969827527 |
| 0.2228711825781372 | 0.7803125646837775 | 0.1547493243872313 |
| 0.7261692981114661 | 0.2792167401775157 | 0.6627927499340823 |
| 0.2283625740735150 | 0.0792738011968224 | 0.8641191343504736 |
| 0.7299608505603031 | 0.5793897439406540 | 0.3287580055735856 |
| 0.9279626814275048 | 0.0783033378889587 | 0.1571047071223830 |
| 0.4320516303163144 | 0.5699635520392895 | 0.6637368718992568 |
| 0.6938557485457972 | 0.2532832815514814 | 0.3259751850229296 |
| 0.2053380218155273 | 0.7427518932054107 | 0.8225924840988069 |
| 0.4008660776672958 | 0.2547580754133810 | 0.6340251438410038 |
| 0.8978224674476779 | 0.7501102281597593 | 0.1436226367227834 |
| 0.4069813382788309 | 0.5501501917253139 | 0.3372246313170488 |
| 0.8957474994694371 | 0.0459238502901598 | 0.8309940924914244 |
| 0.1694989446946358 | 0.6670192462506829 | 0.3920290188046141 |
| 0.6582238053621050 | 0.1592548752672307 | 0.9006864445677295 |
| 0.4614428703748484 | 0.0151257095687428 | 0.7412146376443429 |
| 0.9696633633043013 | 0.5093676163318350 | 0.2420291806198609 |
| 0.8072849463346221 | 0.3143325077927430 | 0.0895633529466428 |
| 0.3376658496931255 | 0.8094922381464595 | 0.5924602912999005 |
| 0.4581654116106767 | 0.6563995467324456 | 0.0977258838908437 |
| 0.9661141235292130 | 0.1731891705531211 | 0.5764610693239431 |
| 0.1627713790089978 | 0.3154279549305650 | 0.7470264252456331 |
| 0.6580340471759539 | 0.8193113380826650 | 0.2512749290412477 |
| 0.8153223714909043 | 0.0179093765523610 | 0.3943530137105281 |
| 0.3147973237262722 | 0.5075123866941790 | 0.9026144352798973 |
| 0.0072986436049351 | 0.8585717157483457 | 0.3007189133051173 |
| 0.5054492992298053 | 0.3511680430813157 | 0.8072108614558102 |
| 0.8562720830134615 | 0.3730696981448316 | 0.4428137274164760 |
| 0.3731855018297410 | 0.8624962546929117 | 0.9446929762847844 |
| 0.0083432030008879 | 0.2195447680310479 | 0.9399570667744779 |
| 0.5206023112674757 | 0.7012515858437423 | 0.4439241778323985 |
| 0.6237497202864216 | 0.4759616708956574 | 0.1895306685428257 |
| 0.1275310862800324 | 0.9573549079754503 | 0.6713123838214665 |
| 0.1140595032890069 | 0.6143954140292014 | 0.0457887836200248 |
| 0.6078812268637870 | 0.1113604228952879 | 0.5397789953848010 |
| 0.2576717940161634 | 0.4664690720181623 | 0.5469633138207960 |
| 0.7550410943113374 | 0.9623332421170339 | 0.0498201701670902 |
| 0.0693452834365851 | 0.6469932657473406 | 0.2574165313196543 |
| 0.5724033055972818 | 0.1492007856044283 | 0.7472422614796297 |
| 0.8384257326560911 | 0.3974243010551000 | 0.2307873465965235 |
| 0.3161507887962228 | 0.9114143663858522 | 0.7463367060233687 |
| 0.8025484906056560 | 0.1658683612734502 | 0.9977264366422927 |
| 0.3052250205522306 | 0.6702602889853236 | 0.5034971578633438 |
| 0.0770434010699957 | 0.1692966406568968 | 0.7293298365004941 |
| 0.5522916811822979 | 0.6927110007085957 | 0.2255547506509829 |

| | | |
|--------------------|--------------------|--------------------|
| 0.2984178660384232 | 0.4196826044824966 | 0.7557739799048302 |
| 0.7983594543658973 | 0.9216423071456112 | 0.2553467485702512 |
| 0.3201681272874294 | 0.6607613809500181 | 0.9896205180157099 |
| 0.8066194688779663 | 0.1687145735416349 | 0.4942457327014095 |
| 0.1672879155999319 | 0.3435345692177749 | 0.2062864712154589 |
| 0.4274984991053255 | 0.3620571706209184 | 0.2680602725736285 |
| 0.4164746672772739 | 0.3887093147058802 | 0.1221894501858187 |
| 0.2858574611815400 | 0.4464684313544088 | 0.2342957502685409 |
| 0.1197274008518254 | 0.3885337538711304 | 0.3683233742461944 |
| 0.0913525992039186 | 0.2476864334329557 | 0.4740836931149429 |
| 0.1431914416023854 | 0.3223657783449952 | 0.5195753003418385 |
| 0.2994534261969256 | 0.2931991943833488 | 0.0928786561318258 |
| 0.4378994251414692 | 0.0613142373899017 | 0.2589460047557754 |
| 0.5210128688429773 | 0.1390700448406853 | 0.2698824459773278 |
| 0.4954493473291903 | 0.1730994596573942 | 0.1298774627268378 |
| 0.4215963354095248 | 0.1432715379466007 | 0.4633132556264913 |
| 0.3581982198738784 | 0.0448523300214371 | 0.4631661718213900 |
| 0.2772980134564401 | 0.1280746732840395 | 0.5742774751275854 |
| 0.2275932358443759 | 0.1859322452311613 | 0.2157382664947812 |
| 0.3681811064910884 | 0.3704817771954902 | 0.2197466418501891 |
| 0.1544725428014359 | 0.3066643492762913 | 0.4355568006908039 |
| 0.2736770231510571 | 0.2301925077223987 | 0.3916130001032649 |
| 0.3367636620493036 | 0.2494245378675193 | 0.2597680595219851 |
| 0.2510804940133911 | 0.2694732032970958 | 0.1902623188978999 |
| 0.4545053924077844 | 0.1494742841611361 | 0.2287675597246968 |
| 0.3329238569806669 | 0.1323515193464463 | 0.4804084713827866 |

Type A isomerisation, configuration R7 of the reactant

1.0000000000000000

| | | |
|---------------------|---------------------|--------------------|
| -7.9236879999800003 | -0.0000170000000000 | 9.8763219999890008 |
| 3.9615609999979999 | -6.8622589999810000 | 9.8761060000119993 |
| 3.9615470000010000 | 6.8621979999780001 | 9.8760699999810004 |

| Si | Al | O | H | C | |
|----|----|----|----|---|--|
| 23 | 1 | 48 | 15 | 7 | |

Direct

| | | |
|--------------------|--------------------|--------------------|
| 0.1196045361437376 | 0.7486670641466495 | 0.2695913237189424 |
| 0.6207564142310031 | 0.2474817229047819 | 0.7662618544065778 |
| 0.8513286548137942 | 0.4758092690330510 | 0.3083276503407413 |
| 0.3476469172751615 | 0.9775650137022257 | 0.8172543467079276 |
| 0.8907736296550067 | 0.2018269551711579 | 0.0409586227537988 |
| 0.3992118995822902 | 0.6968693740236369 | 0.5454076783535549 |
| 0.7428998891288644 | 0.3701750773289509 | 0.2037570153951957 |
| 0.2460902499580144 | 0.8697294307263304 | 0.7026326927597558 |
| 0.0146251937153837 | 0.6441745513846201 | 0.1619478965225065 |
| 0.5128793336097230 | 0.1426184353930706 | 0.6643050959080984 |
| 0.2876537970226003 | 0.5981266433163743 | 0.4408053174173930 |
| 0.7936792558358791 | 0.0919759525873714 | 0.9369913930485421 |
| 0.2860912844831860 | 0.3717996249058719 | 0.6660860183039938 |
| 0.7831861029468455 | 0.8724787418486288 | 0.1630900232390232 |
| 0.7414137457594018 | 0.1444513830032871 | 0.4325835520251844 |
| 0.2420046664903228 | 0.6457460826511781 | 0.9311580166881142 |
| 0.3981832596556411 | 0.4735881541481859 | 0.7725781483933306 |
| 0.8916844560309242 | 0.9767435075275729 | 0.2692997666907586 |
| 0.1245836890551722 | 0.2045018810332391 | 0.8113368618438507 |
| 0.6231649133029981 | 0.7029347962249094 | 0.3078135903199941 |
| 0.3460454821737486 | 0.7517403227036721 | 0.0402796163196304 |
| 0.8422559077504136 | 0.2530355994393629 | 0.5383679362411808 |
| 0.5161995554706991 | 0.5980721393855778 | 0.2074091025016130 |

| | | |
|--------------------|--------------------|--------------------|
| 0.0223412579529321 | 0.0945794722793645 | 0.7073452302686631 |
| 0.2247046292181965 | 0.7911475522500672 | 0.1477964408687804 |
| 0.7116779610276640 | 0.2983601871795256 | 0.6347584310459023 |
| 0.2352366092871387 | 0.0898249121899718 | 0.8581138403249408 |
| 0.7352734019133771 | 0.5875955156675229 | 0.3440460995037562 |
| 0.9327710928774889 | 0.0866535128084045 | 0.1529446822230786 |
| 0.4433885638395422 | 0.5799477776137081 | 0.6535232979320310 |
| 0.7018035915408174 | 0.2601491509721554 | 0.3207868147898086 |
| 0.2045328349745878 | 0.7577757024008194 | 0.8176622453494475 |
| 0.4019564578135283 | 0.2604042303684893 | 0.6256497751528278 |
| 0.9018113816889392 | 0.7605983139175677 | 0.1281521140840084 |
| 0.4120852037472319 | 0.5621550465700738 | 0.3343023787180844 |
| 0.9233541909337811 | 0.0457365034114902 | 0.8478449031539116 |
| 0.1740058992165507 | 0.6741953938031909 | 0.3846147220481232 |
| 0.6865182225314714 | 0.1696625108803129 | 0.8712933423228330 |
| 0.4682471704220151 | 0.0218662688815761 | 0.7329615893705699 |
| 0.9725411796433049 | 0.5210326479716402 | 0.2333257654754277 |
| 0.8197536117043486 | 0.3238257089989513 | 0.0848411969599595 |
| 0.3401908611835564 | 0.8182002388992446 | 0.5876204611984248 |
| 0.4596443548906468 | 0.6690077687110664 | 0.0948254143770043 |
| 0.9507813024782975 | 0.1808704593236501 | 0.5957639398833815 |
| 0.1670962092480956 | 0.3278623912607448 | 0.7506447325545123 |
| 0.6640893686322231 | 0.8254881941185057 | 0.2430296211734298 |
| 0.8129061684339202 | 0.0228584843163808 | 0.3889908305202233 |
| 0.3189104977567720 | 0.5225836939580039 | 0.8905623452189919 |
| 0.0116624590192733 | 0.8683667922296407 | 0.2976228263771108 |
| 0.5143616470716244 | 0.3636068806050954 | 0.8061940030156226 |
| 0.8753082695408450 | 0.3725982740643712 | 0.4308563849222359 |
| 0.3776430604235854 | 0.8727387083753402 | 0.9387372913020275 |
| 0.0103263630320752 | 0.2234382092164446 | 0.9310167107263972 |
| 0.5154336738658000 | 0.7181343951157553 | 0.4302426118398758 |
| 0.6191870911531323 | 0.4751101331420866 | 0.1815801997313756 |
| 0.1342535236245432 | 0.9722144366313860 | 0.6585321376607729 |
| 0.1201126739635574 | 0.6229924129482595 | 0.0389361268162322 |
| 0.6192777540016098 | 0.1233224317649112 | 0.5404692462802417 |
| 0.2606755240750688 | 0.4735038503997902 | 0.5407109567765379 |
| 0.7512472473891150 | 0.9761102820445116 | 0.0437699292971587 |
| 0.0678123859763333 | 0.6615188077284296 | 0.2496746701333290 |
| 0.5609589861378866 | 0.1625993556913700 | 0.7534477347628634 |
| 0.8273397821525086 | 0.4222438199213681 | 0.2263655324303577 |
| 0.3195805492551602 | 0.9217903541199587 | 0.7405553095832831 |
| 0.7959260630570313 | 0.1783588857322904 | 0.0033181913860597 |
| 0.3028523690422286 | 0.6773163473170882 | 0.5048735523715662 |
| 0.0938442060014219 | 0.1832600458032614 | 0.7129220444460963 |
| 0.5763420606163078 | 0.6845143708254545 | 0.2163241786206276 |
| 0.3149464449830194 | 0.4272386632580191 | 0.7424115314620221 |
| 0.8071905696417409 | 0.9269768027647325 | 0.2443691212863580 |
| 0.3250198985014771 | 0.6720418715986124 | 0.9817900010565518 |
| 0.8295909838114225 | 0.1690651982086850 | 0.4770402454716122 |
| 0.3893368591208907 | 0.3438493661378093 | 0.3596695900679248 |
| 0.3567151663310107 | 0.1438055559857616 | 0.5238750249513933 |
| 0.3950710490644887 | 0.0150984950409060 | 0.4736154709164861 |
| 0.5062660488977220 | 0.0896227556103526 | 0.4319202991142062 |
| 0.1341640499421816 | 0.3834230174871744 | 0.3372754033981998 |
| 0.0853208470780741 | 0.2934054374658108 | 0.4860451909245576 |
| 0.2101478106280661 | 0.3550212341029716 | 0.4415566280948250 |
| 0.5211874494319215 | 0.2759793581181839 | 0.2590881857749122 |
| 0.5491322079444615 | 0.1076146804629083 | 0.2085243604298868 |

| | | |
|--------------------|--------------------|--------------------|
| 0.4266341448191761 | 0.1747525938486752 | 0.1448017987800008 |
| 0.4387699581791330 | 0.0318987723466300 | 0.2608375554905442 |
| 0.1009838622333858 | 0.1704804251486044 | 0.3718344633882421 |
| 0.1834658113406102 | 0.0636693233343139 | 0.4709314722952644 |
| 0.2496934903993263 | 0.0707661292080865 | 0.3130029130930189 |
| 0.3914076146286206 | 0.3718730252899456 | 0.2082076859438038 |
| 0.4097096113218575 | 0.1028248110917261 | 0.4492357542582749 |
| 0.1672863092909882 | 0.3139270459907758 | 0.4153082569662651 |
| 0.2492833605054646 | 0.2111639900876444 | 0.3685845882425537 |
| 0.3815379171355558 | 0.1901978923899099 | 0.3251628206544943 |
| 0.4217511303099467 | 0.3029992857466809 | 0.2863380781291889 |
| 0.4519013758159685 | 0.1216293299021198 | 0.2293302530677840 |
| 0.1950814619217688 | 0.1259836631781356 | 0.3754471440838656 |

Type A isomerization, configuration TS7 of the TS

1.0

| | | |
|-----------------|-----------------|----------------|
| -7.923687999980 | -0.000017000000 | 9.876321999989 |
| 3.961560999998 | -6.862258999981 | 9.876106000012 |
| 3.961547000001 | 6.862197999978 | 9.876069999981 |

Si Al O H C

23 1 48 15 7

direct

| | | |
|----------------|----------------|----------------|
| 0.120370783341 | 0.752307785373 | 0.269754140390 |
| 0.620810090349 | 0.242781390865 | 0.768053412189 |
| 0.853536492994 | 0.472813697026 | 0.308727072882 |
| 0.344029245556 | 0.979200848700 | 0.816826375254 |
| 0.886939504293 | 0.205221825879 | 0.037498237528 |
| 0.402301135353 | 0.694892898509 | 0.548573170510 |
| 0.747435642288 | 0.373291373879 | 0.199404209333 |
| 0.242989711605 | 0.864911501681 | 0.707896918033 |
| 0.016530071212 | 0.643140051772 | 0.166700599619 |
| 0.512176222154 | 0.143846645441 | 0.659341207620 |
| 0.290048389983 | 0.599098573970 | 0.438446433016 |
| 0.786857557318 | 0.093648148085 | 0.939894228694 |
| 0.281221397384 | 0.375562605478 | 0.666395747093 |
| 0.787314042946 | 0.870672649272 | 0.163950152308 |
| 0.734355870845 | 0.149010959105 | 0.429270017667 |
| 0.246400558615 | 0.639999600097 | 0.936263061474 |
| 0.392508527956 | 0.471029041232 | 0.775938966657 |
| 0.894236372218 | 0.981212830283 | 0.266252457905 |
| 0.121772330457 | 0.204314017947 | 0.806276833817 |
| 0.622666365773 | 0.703715819795 | 0.312023203213 |
| 0.348584745135 | 0.752320854196 | 0.039016179947 |
| 0.841076277944 | 0.252311920213 | 0.540872976615 |
| 0.516177948929 | 0.603194873817 | 0.207665707056 |
| 0.020365314935 | 0.092040849455 | 0.704485382739 |
| 0.226000642199 | 0.789820407382 | 0.146047237656 |
| 0.719779412207 | 0.296969450242 | 0.647121567636 |
| 0.230768637148 | 0.091135066031 | 0.857837125803 |
| 0.733233422535 | 0.583092831108 | 0.338968151971 |
| 0.932481600938 | 0.092018687931 | 0.148976650405 |
| 0.440925629116 | 0.576874508679 | 0.658632995381 |
| 0.701120846494 | 0.264088124985 | 0.314073340370 |
| 0.207698449734 | 0.750024732518 | 0.822649933739 |
| 0.401550247180 | 0.265959131541 | 0.629214338643 |
| 0.905818139528 | 0.759614445182 | 0.127526666952 |
| 0.411707387011 | 0.559089045214 | 0.330681748618 |
| 0.913911533935 | 0.057333287997 | 0.843662463557 |

| | | |
|----------------|----------------|----------------|
| 0.175606191698 | 0.680316517353 | 0.384208893601 |
| 0.672380790008 | 0.166147241214 | 0.883670436891 |
| 0.462970395347 | 0.025929726337 | 0.729983200695 |
| 0.972271855280 | 0.521664459110 | 0.237742555796 |
| 0.818899951775 | 0.329047130279 | 0.078711411753 |
| 0.338521400312 | 0.815902039800 | 0.591560422326 |
| 0.463173721255 | 0.673419790964 | 0.092695164658 |
| 0.956668083186 | 0.171884548659 | 0.586546036975 |
| 0.163613326519 | 0.328065667395 | 0.745359604072 |
| 0.669001982312 | 0.823007100450 | 0.247587945478 |
| 0.813810113994 | 0.027995658564 | 0.385491417646 |
| 0.321311090990 | 0.515701064719 | 0.897181320734 |
| 0.015630767500 | 0.875247526680 | 0.294121924142 |
| 0.506035416444 | 0.355057170092 | 0.804857873512 |
| 0.871340076123 | 0.373250982440 | 0.434592820313 |
| 0.376551099771 | 0.875011249430 | 0.937494649365 |
| 0.003510320767 | 0.225152817147 | 0.922381416712 |
| 0.523031895139 | 0.716780468186 | 0.439654780547 |
| 0.627065489501 | 0.485290342433 | 0.179657518608 |
| 0.127048392356 | 0.961943247178 | 0.669751379064 |
| 0.126043413873 | 0.618438481555 | 0.047097984692 |
| 0.607505363039 | 0.126846080492 | 0.528883860100 |
| 0.259718609504 | 0.476275207719 | 0.539285697891 |
| 0.753433774374 | 0.972734623163 | 0.044980754184 |
| 0.064315411697 | 0.664961905645 | 0.255768802143 |
| 0.575970719508 | 0.155291758039 | 0.740355887321 |
| 0.839154606498 | 0.414007719002 | 0.224453782251 |
| 0.315668877314 | 0.921605516728 | 0.742122355502 |
| 0.787838049026 | 0.179392387989 | 0.007970282831 |
| 0.312556937980 | 0.675923290889 | 0.499228844489 |
| 0.097509830723 | 0.178917545042 | 0.705882099170 |
| 0.562850506042 | 0.695579435953 | 0.224777491386 |
| 0.300809651398 | 0.434689561476 | 0.746416712816 |
| 0.812091131402 | 0.927452840713 | 0.242677951675 |
| 0.332388774041 | 0.668523219930 | 0.981409877100 |
| 0.810285896251 | 0.176449707800 | 0.485049280526 |
| 0.378239622024 | 0.359950138527 | 0.343831809106 |
| 0.269573821641 | 0.141541234943 | 0.545405625640 |
| 0.384822964464 | 0.021103003763 | 0.481138935837 |
| 0.420712052761 | 0.147130995038 | 0.480668772212 |
| 0.144658442351 | 0.370133611788 | 0.312192961288 |
| 0.094233336518 | 0.286835908158 | 0.466042484256 |
| 0.204203921605 | 0.362749021968 | 0.421168928237 |
| 0.528040118384 | 0.278305042417 | 0.276307796522 |
| 0.574780771223 | 0.079920187064 | 0.265051728144 |
| 0.503285463996 | 0.147403721984 | 0.149092086951 |
| 0.464394103454 | 0.021699627455 | 0.272753965209 |
| 0.183251197040 | 0.155555833653 | 0.283640336985 |
| 0.147208852219 | 0.091436074863 | 0.443818254449 |
| 0.289957105845 | 0.025363624774 | 0.349000674153 |
| 0.423694297913 | 0.363880481419 | 0.189520456841 |
| 0.354245663167 | 0.117476775965 | 0.473689789004 |
| 0.173556954633 | 0.311129299274 | 0.393996054266 |
| 0.269973185095 | 0.199212327965 | 0.364558116233 |
| 0.393468163902 | 0.197147899386 | 0.309736538715 |
| 0.432536631831 | 0.305751669278 | 0.280423743314 |
| 0.488204623790 | 0.104469315154 | 0.247622174844 |
| 0.221288893094 | 0.110837361665 | 0.360919996316 |

Type A isomerisation, configuration P7 of the product

1.000000000000000000
-7.9236879999800003 -0.0000170000000000 9.8763219999890008
3.9615609999979999 -6.8622589999810000 9.8761060000119993
3.9615470000010000 6.8621979999780001 9.8760699999810004

Si Al O H C
23 1 48 15 7

Direct

0.1196601935143533 0.7478529107366956 0.2745032450138981
0.6201643506498387 0.2373167283563844 0.7754095532571116
0.8495816676838095 0.4713241751884258 0.3132899273668039
0.3423649291449224 0.9756028290646717 0.8193985863212201
0.8862830224785369 0.2022341327169418 0.0422678350791111
0.4022769658430718 0.6932675094063919 0.5503485764271634
0.7448395023712986 0.3693003140228304 0.2057725665673174
0.2415540788924140 0.8627595753931575 0.7106216299127639
0.0163283928126515 0.6380224653100032 0.1708906807198952
0.5120273072212809 0.1406015291634701 0.6652276691590246
0.2893438369017725 0.5937789946524535 0.4413101336194426
0.7839765718303332 0.0941096266273547 0.9413655380335050
0.2806141428112577 0.3736137300228644 0.6724933337369139
0.7862088211625540 0.8688605509245000 0.1675287730971393
0.7312775116487743 0.1479359865517004 0.4333912241412651
0.2437825816490846 0.6372681081501127 0.9403028540711115
0.3916859597397390 0.4703409888271254 0.7786337620250379
0.8908838499853040 0.9781701652715022 0.2715373370638031
0.1195234992895908 0.2022132188150161 0.8102271140533499
0.6177676188206233 0.7052373816019897 0.3136457563785534
0.3460939254659323 0.7501027770369056 0.0440670132973207
0.8420222998305315 0.2510034061352034 0.5437688509039924
0.5124508674167016 0.6007308759970225 0.2115592294910875
0.0189897289626208 0.0955994617508272 0.7007134411035559
0.2263657195066210 0.7884076002134242 0.1532669360042565
0.7275942676598970 0.2837817382847259 0.6606535967284661
0.2266569288712024 0.0854894069138604 0.8609980419681588
0.7301464875764188 0.5851134528179665 0.3331171863180188
0.9309283626851603 0.0877164701171890 0.1533662648316729
0.4398979008354986 0.5765733040248942 0.6620987199131786
0.6940808828858871 0.2609618698299457 0.3179505241836978
0.2078989745307572 0.7465661372224072 0.8255606900583934
0.4037092487733838 0.2657475485635223 0.6376410102823290
0.9054850782179459 0.7568430296909826 0.1360598271269612
0.4069048533532452 0.5518756943109305 0.3306021479175403
0.9031549052428018 0.0679600679638254 0.8342314423387835
0.1725520524525265 0.6767165891981661 0.3906642145233454
0.6599580011088322 0.1652428190891277 0.8992225470487737
0.4602442432049250 0.0245319694551086 0.7357433134482232
0.9694282510266324 0.5183660487052891 0.2422965555057217
0.8158581474899675 0.3255244623322783 0.0845682873780179
0.3321376967623114 0.8139968516388929 0.5931913569953211
0.4631310580522281 0.6692593042612008 0.0940267174168927
0.9659552661912890 0.1719661660481092 0.5748958744814822
0.1648371990815245 0.3235851146600921 0.7521089406279751
0.6649205633998148 0.8244738178185413 0.2450427555390585
0.8138500278473342 0.0266893173599683 0.3900208688071015
0.3239064214050549 0.5123723323959840 0.9020848817434616
0.0107983626519600 0.8687307189883204 0.2983922916327844

| | | |
|--------------------|--------------------|--------------------|
| 0.5054273349829915 | 0.3531921728350931 | 0.8038378250160175 |
| 0.8594961804479555 | 0.3797906241219001 | 0.4443776449203678 |
| 0.3741087960965022 | 0.8716537805191942 | 0.9407858194378479 |
| 0.0027974830440835 | 0.2231868808001453 | 0.9279573367443358 |
| 0.5246557941185891 | 0.7169621371220779 | 0.4445197966197716 |
| 0.6277367841700736 | 0.4854667783880482 | 0.1839046257198451 |
| 0.1235025162576870 | 0.9602605626677750 | 0.6782035943662618 |
| 0.1221772148690652 | 0.6137033938416193 | 0.0486053680795014 |
| 0.6068928822546396 | 0.1226165986896139 | 0.5352421538820992 |
| 0.2589534468832639 | 0.4722948762929413 | 0.5446607147889052 |
| 0.7601180894587907 | 0.9686309496587383 | 0.0444164544521967 |
| 0.0707343974834443 | 0.6570673476807141 | 0.2564824117546727 |
| 0.5784317299378867 | 0.1484923509028093 | 0.7464832533347826 |
| 0.8384904618490376 | 0.4047215021330418 | 0.2337216750820549 |
| 0.3186129294345532 | 0.9162917238736267 | 0.7429147888221299 |
| 0.7878447359861521 | 0.1767912541519024 | 0.0110966428882504 |
| 0.3191994078386975 | 0.6697864383920800 | 0.4967419213549886 |
| 0.0914182348162575 | 0.1823276404104682 | 0.7092019073747950 |
| 0.5498235770628171 | 0.6967533396362129 | 0.2337927782333711 |
| 0.2961394016298918 | 0.4373702762198693 | 0.7513513287255440 |
| 0.8046735978940774 | 0.9280923458407061 | 0.2487416996371444 |
| 0.3253541943043716 | 0.6656135817979153 | 0.9908439907202508 |
| 0.8053639448762332 | 0.1815689450160994 | 0.4859358754857879 |
| 0.3775362505393070 | 0.4134437886450000 | 0.2335086184371854 |
| 0.2625038156685545 | 0.1864117765472243 | 0.5292756219334982 |
| 0.4213784176685716 | 0.1162497527990328 | 0.4673880257706217 |
| 0.3632325384153977 | 0.2783793682709207 | 0.4396541985655200 |
| 0.1678128169112509 | 0.3358673952506717 | 0.2498611443695235 |
| 0.1139193723500802 | 0.2933110494686605 | 0.4112731182729422 |
| 0.1991300719756650 | 0.3990839833450552 | 0.3322283962804414 |
| 0.5202368202572332 | 0.3530549474102342 | 0.1301306440431327 |
| 0.6068867535091130 | 0.1439318538033124 | 0.2022059455404848 |
| 0.5281496194125920 | 0.1280648847938773 | 0.1277804657039987 |
| 0.5177461059384649 | 0.0365954439368385 | 0.2811142925743363 |
| 0.2658661394637689 | 0.0889538641812049 | 0.2866906011839725 |
| 0.1965503934207093 | 0.0840930173584621 | 0.4425751872732580 |
| 0.3527411674792115 | 0.0086296625597418 | 0.3925061355270397 |
| 0.3774820916674479 | 0.3850429654236168 | 0.1090753383617297 |
| 0.3441213055692393 | 0.1965626558878962 | 0.4512788363830184 |
| 0.1901669342067036 | 0.3162280705413837 | 0.3325438036848480 |
| 0.3041039669982928 | 0.2083691656715564 | 0.3412065823768918 |
| 0.4160379335385587 | 0.2274834510954735 | 0.2475924023802098 |
| 0.4263262653154115 | 0.3505283004025512 | 0.1778316479546492 |
| 0.5222653557068963 | 0.1264829351297635 | 0.2187646966405309 |
| 0.2797319487458685 | 0.0897352745894156 | 0.3666242885981776 |