

Supporting Information for

“Quantum Chemical Investigation of the thermal rearrangement of *cis*- and *trans*-pinane”

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CASSCF(4,4) / 6-31G(d,p) optimized structures xyz-coordinates for:

reactants:

cis-pinane (1)

C	-0.01165300	-0.34190600	-1.01971800
C	1.04830300	-0.36656900	0.17907500
C	2.42130600	-0.83792200	-0.32163100
C	0.91167700	1.17925700	0.14829400
C	-0.32585000	1.67125100	0.90414100
C	-1.60364100	0.83689400	0.59659300
C	-1.47360000	-0.17911400	-0.57798300
C	0.52822400	1.05991500	-1.37241100
C	0.76612200	-1.10830800	1.48718900
C	-2.17829000	-1.50354100	-0.27150700
H	1.79019200	1.76178600	0.41346700
H	0.08389400	-1.12371400	-1.76884200
H	-0.13691100	1.66144400	1.97417900
H	-0.48858700	2.71198000	0.63640800
H	-1.89064100	0.29620400	1.49139100
H	-2.43218100	1.50780700	0.39324700
H	1.38319800	1.05222200	-2.03428200
H	-0.19476300	1.77749400	-1.74860000
H	0.76146200	-2.18276700	1.32470300
H	1.55426400	-0.89475900	2.20538400
H	-0.17193000	-0.84259800	1.95090500
H	3.18723500	-0.62165800	0.41873600
H	2.41550300	-1.91267000	-0.48350900
H	2.72496500	-0.37096600	-1.24994100
H	-1.98527800	0.24438800	-1.44047500
H	-3.22197200	-1.33270000	-0.02089100
H	-2.15195100	-2.16290200	-1.13474600
H	-1.72209200	-2.02833400	0.56062000

trans-pinane (2)

C	0.01682300	-0.18598300	-1.59430300
C	-0.10652400	-0.93850100	-0.25048500
C	-1.32763200	-0.42957000	0.53095400
C	-1.54092500	1.08734000	0.27235600
C	-0.27115600	1.85798800	-0.17263500
C	0.75637600	0.92353000	-0.81763300
C	1.22788400	-0.19703400	0.21134500
C	2.48632500	-0.92930500	-0.26655200
C	1.41839300	0.17029000	1.68222700
C	-2.59124000	-1.22000100	0.18167600
H	-1.13842300	-0.58852900	1.58881700
H	1.53878200	1.47802600	-1.32801700
H	-0.07272300	-2.02470300	-0.26785200
H	0.18161100	2.38506100	0.66119500
H	-0.55971400	2.62230100	-0.88987000
H	-1.97705200	1.55390900	1.15100500
H	-2.28573800	1.18863600	-0.51109700
H	0.64660300	-0.69797000	-2.30888200
H	-0.90222000	0.09233200	-2.09889900
H	1.57104500	-0.72614600	2.27824200
H	2.30134500	0.79349400	1.80119400
H	0.58364000	0.70704100	2.11213200
H	3.36103200	-0.29435600	-0.15132300
H	2.65105100	-1.82541300	0.32628200
H	2.43795700	-1.23113800	-1.30551100
H	-3.45479300	-0.82737100	0.71183600
H	-2.80748800	-1.17082300	-0.88241300
H	-2.48485400	-2.26687800	0.45146500

products:

β -citronellene ((-)-3)

C	-1.75130000	1.05294400	-0.38180200
C	-2.08590300	2.18999700	0.24114300
C	1.18328700	0.23027800	0.67498100
C	2.32784400	0.10917300	-0.02187800
C	3.13453100	1.32853700	-0.40345700
C	0.27232400	-0.88698600	1.13304700
C	-0.85503600	-1.27201600	0.15540200
C	-2.07622200	-0.33598700	0.11560700
C	2.91872800	-1.19954800	-0.49109600
C	-3.18069000	-0.95169400	-0.75707500
H	0.86518100	1.22622900	0.93213100
H	-1.24611900	1.10796100	-1.33510500
H	0.85889200	-1.77713100	1.33393900
H	-0.17063100	-0.60602300	2.08630700
H	-0.44335400	-1.37100800	-0.84756000
H	-1.21517600	-2.25992600	0.43477100
H	-1.85682800	3.15242400	-0.18171600
H	-2.59440900	2.18704500	1.19086700
H	3.03108600	-1.19694600	-1.57298500
H	3.91236000	-1.34258700	-0.07208400
H	2.31811200	-2.05907500	-0.22575900
H	4.14007700	1.27327200	0.00829900
H	3.23967600	1.40385400	-1.48371800
H	2.67583400	2.24335600	-0.04630700
H	-2.46245800	-0.24783200	1.13000300
H	-3.45999800	-1.93743600	-0.39644000
H	-4.06818600	-0.32750600	-0.75668700
H	-2.84943800	-1.05687200	-1.78719100

β -citronellene ((+)-3)

C	1.66414600	1.02578300	0.77745600
C	2.05024000	-0.41581100	0.51928800
C	0.83548500	-1.36951400	0.54323600
C	-0.17031800	-1.29296800	-0.62134500
C	-1.00902300	-0.03691400	-0.67576800
C	-2.23996400	0.14624700	-0.16449200
C	-3.02962300	-0.89926500	0.58747500
C	-2.94821200	1.47300200	-0.31109900
C	2.09253400	2.11224900	0.12138200
C	2.92464300	-0.61115000	-0.72190600
H	2.65329000	-0.71528100	1.37803200
H	-0.55328500	0.80289600	-1.17305700
H	0.99439900	1.16980600	1.61183800
H	-0.81230600	-2.16460200	-0.55312500
H	0.35918100	-1.39734600	-1.56447500
H	0.29714900	-1.22242300	1.47725300
H	1.22559300	-2.38491100	0.57544600
H	1.77056800	3.09539900	0.41674700
H	2.76162700	2.06043200	-0.71863500
H	-3.28614600	-0.53646400	1.58026200
H	-3.96726400	-1.11006900	0.07782500
H	-2.49804700	-1.83356400	0.70703400
H	-3.89179800	1.35323600	-0.83936500
H	-3.18333300	1.89851100	0.66220200
H	-2.34785300	2.19260800	-0.85559700
H	3.15900800	-1.66270800	-0.85762700
H	2.43637800	-0.25957500	-1.62486600
H	3.86339100	-0.07590000	-0.62526000

isocitronellene ((-)-4)

C	-0.78183500	-0.01850700	0.51585700
C	0.00318500	-1.27795600	0.20808600
C	0.98559700	-1.12124100	-0.97539000
C	2.24387500	-0.26280000	-0.76725400
C	2.00035100	1.20849300	-0.54872600
C	2.57975000	1.94781700	0.40580600
C	-1.99489000	0.33193000	0.05136800
C	-2.63623800	1.63337400	0.47496900
C	-2.82856600	-0.48317600	-0.90953200
C	0.69329900	-1.79576300	1.47652600
H	-0.69698000	-2.04835400	-0.09985100
H	1.31955200	-2.11791900	-1.25828500
H	0.43379400	-0.73366900	-1.82922900
H	2.85259300	-0.37343900	-1.66399600
H	2.84118900	-0.65792900	0.04903000
H	-3.04320000	0.09459000	-1.80575500
H	-3.78715300	-0.73692000	-0.46230800
H	3.25657600	1.51639400	1.12442900
H	1.33163600	1.68932100	-1.24656200
H	-2.35157900	-1.40303200	-1.21900700
H	-0.29408600	0.67212500	1.18461200
H	2.39168700	3.00358100	0.49176200
H	-2.83466600	2.26809100	-0.38610300
H	-3.59258500	1.45434000	0.96185900
H	-2.00822700	2.18766800	1.16277300
H	1.26972900	-2.69369400	1.27080500
H	1.36665700	-1.05598700	1.89813500
H	-0.04210500	-2.03819200	2.23743400

isocitronellene ((+)-4)

C	-1.65586900	-0.68976800	-0.01094300
C	-0.68577200	-0.14221000	-0.76725800
C	2.77869400	-1.71567900	-0.46895000
C	2.17222000	-0.95446500	0.45048900
C	0.03845100	1.19216600	-0.61907700
C	0.94320600	1.29942800	0.62746100
C	2.27896900	0.54599100	0.53347500
C	-2.24276200	-2.03295100	-0.38384400
C	-2.26250900	-0.09214100	1.23770100
C	-0.91371900	2.39436300	-0.73035300
H	1.17748100	2.34948700	0.78880700
H	0.40771200	0.97036800	1.51302700
H	2.86243600	0.79891300	1.41808500
H	-0.34903800	3.31919400	-0.80978300
H	2.84292500	0.91563100	-0.31988900
H	-2.17236100	-0.78806700	2.06888800
H	-1.56945200	2.48422300	0.12814700
H	0.70054200	1.26068600	-1.47999200
H	-3.32563000	0.08711300	1.09253700
H	-1.53877900	2.30793000	-1.61335800
H	3.38128400	-1.28637800	-1.25194500
H	1.57942400	-1.43298800	1.21504000
H	-1.80848900	0.83977700	1.53775900
H	-0.37280200	-0.71999200	-1.62154700
H	2.68637100	-2.78749300	-0.46194600
H	-2.09464500	-2.75673300	0.41487700
H	-3.31607900	-1.95614500	-0.54471100
H	-1.79634100	-2.43393500	-1.28620000

1a-g-path: gauche 1 → (-)-3

1a-g-TS1

C	1.03960500	-1.25040800	0.05231100
C	-1.59315900	0.00091500	-0.35562200
C	-2.35315700	-1.24290000	-0.75319000
C	-0.86676700	0.02002700	0.98336900
C	0.08035900	1.22420400	1.14250300
C	1.18027600	1.24822100	0.07610100
C	1.97290400	-0.06721500	0.01363300
C	-0.00256000	-1.26835500	1.13666900
C	-2.25038900	1.28097500	-0.81569100
C	2.90387900	-0.10499100	-1.19890100
H	-1.60626900	0.06316100	1.78965000
H	1.42349100	-2.19340500	-0.30595500
H	-0.47344100	2.15728000	1.12295100
H	0.53542100	1.16749500	2.12985600
H	0.73632800	1.42899100	-0.89924800
H	1.86106900	2.07443600	0.26841900
H	-0.61132700	-2.16230200	1.08586300
H	0.46588700	-1.27321000	2.12374700
H	-2.61382900	1.18509300	-1.83379000
H	-3.11212400	1.51988900	-0.18825200
H	-1.58525100	2.13475900	-0.78465100
H	-3.23252900	-1.38018400	-0.11956700
H	-2.70833800	-1.16039700	-1.77542100
H	-1.76093000	-2.14538000	-0.68868300
H	2.59525400	-0.11499500	0.91375100
H	3.57787800	0.74685800	-1.20108500
H	3.50917300	-1.00702200	-1.20132200
H	2.33359800	-0.08391200	-2.12335800

1a-g-IM

C	-1.34514200	-0.98242800	0.63571400
C	-0.12192000	-0.62658900	1.49390600
C	0.92580500	0.30405900	0.84256900
C	0.14629500	1.53878400	0.12207000
C	-1.03467000	1.10210400	-0.66177500
C	-2.04985800	0.26347000	0.06883800
C	1.95365900	-0.34074900	-0.03251400
C	1.56218500	-1.34080700	-1.08495000
C	-3.24789900	-0.10536800	-0.80487200
C	3.21890400	0.43550700	-0.29374800
H	1.47533800	0.77386900	1.65394400
H	-0.92589700	0.94152700	-1.72356600
H	0.36484900	-1.53674600	1.83382500
H	-0.48529500	-0.12733400	2.39078100
H	-1.06269600	-1.62895800	-0.18969000
H	-2.04437400	-1.55137500	1.24526800
H	0.84794400	2.10993900	-0.47514500
H	-0.18204800	2.17891100	0.93835400
H	0.88758800	-0.89935300	-1.82235900
H	2.43371500	-1.70432700	-1.61983300
H	1.05463100	-2.20210000	-0.66420300
H	4.05054500	-0.23404500	-0.49613900
H	3.12209900	1.08823100	-1.16346800
H	3.49194200	1.05977900	0.55116800
H	-2.41426300	0.84503200	0.91815300
H	-3.97544100	-0.68851000	-0.24774100
H	-3.74661200	0.78389900	-1.17824700
H	-2.93617300	-0.69634100	-1.66253500

1a-g-TS2

C	-1.06437000	1.16081300	-0.55479900
C	0.05975900	1.58172500	0.23148900
C	0.97717700	0.14894500	0.87529900
C	1.97895400	-0.31619600	-0.05542400
C	3.23466000	0.50042800	-0.22364800
C	-0.10866100	-0.81450500	1.39433200
C	-1.33500700	-1.05367400	0.49921600
C	-2.06173800	0.24552100	0.10648500
C	1.61165700	-1.20722000	-1.20859700
C	-3.28217000	-0.02830700	-0.77140200
H	1.46535000	0.62076200	1.71887000
H	-0.94009100	1.05474600	-1.62276800
H	0.35000100	-1.77061800	1.63260500
H	-0.46868800	-0.41387700	2.34015200
H	-1.05262600	-1.58333100	-0.40614700
H	-2.02248500	-1.70636400	1.03385000
H	0.77797300	2.20700900	-0.27921900
H	-0.22677200	2.02815400	1.17543500
H	0.92169100	-0.69857900	-1.88729900
H	2.48764400	-1.48730800	-1.78446700
H	1.12469400	-2.12100700	-0.88515000
H	4.09013600	-0.13902800	-0.42581800
H	3.15418700	1.19199000	-1.06421900
H	3.45880000	1.08646400	0.66158800
H	-2.40308300	0.72172700	1.02711800
H	-3.99222200	-0.67674400	-0.26633200
H	-3.79374800	0.89492700	-1.02600600
H	-2.99232300	-0.51409300	-1.69990000

1a-a-path: anti 1 → (-)-3

1a-a-TS1

C	-0.95539900	1.38103100	0.11335100
C	-1.08627300	-0.06612800	-0.30903000
C	0.01093000	-0.87454200	0.50400300
C	-0.33336000	-0.85221200	1.97496500
C	0.39375600	1.98310000	0.42262800
C	1.53807300	1.13292600	-0.13701800
C	1.46653300	-0.34781600	0.28921200
C	-2.50384900	-0.57065600	0.02068500
C	-0.91151100	-0.24317800	-1.83444500
C	2.28654400	-1.23074400	-0.65747800
H	-1.76808400	2.04754700	-0.12769100
H	-0.02769800	-1.91014100	0.15872100
H	0.45708600	2.98824900	0.01220100
H	0.51430200	2.09453800	1.49951100
H	1.53115900	1.20870800	-1.22001900
H	2.49251800	1.54434600	0.18141800
H	-1.29475900	-1.19251300	2.30964700
H	0.45793000	-0.91413600	2.70111900
H	-1.03820600	-1.28562100	-2.11605600
H	-1.66569900	0.33307500	-2.36247300
H	0.05338600	0.08168400	-2.19627400
H	-3.22690300	-0.08842700	-0.63089300
H	-2.58489900	-1.64322700	-0.13792100
H	-2.79542000	-0.35125200	1.03923500
H	1.95617200	-0.41231200	1.25686700
H	3.30176400	-0.85374500	-0.74936500
H	2.34629000	-2.24954400	-0.28533800
H	1.85839400	-1.26791600	-1.65392600

1a-a-IM

C	0.19040000	0.89293200	0.26912500
C	-1.21397800	-0.00871500	0.05459900
C	-2.33863800	0.82119600	-0.57717100
C	-0.91237200	-1.17819100	-0.81677800
C	0.22939700	-2.10057100	-0.47679500
C	1.39496700	-1.33639800	0.18419500
C	1.43242600	0.13426300	-0.24595700
C	0.09935100	2.26338900	-0.28583300
C	-1.66991100	-0.46735800	1.45235600
C	2.72554400	0.80368300	0.22639300
H	-1.18983500	-1.10351300	-1.85578400
H	0.28608000	0.97761700	1.34879900
H	-0.10154300	-2.90765900	0.17518300
H	0.57932800	-2.57711700	-1.38786100
H	1.31668800	-1.37977800	1.26836500
H	2.33478000	-1.81951100	-0.06790600
H	-0.47089000	3.01912700	0.22331000
H	0.30412200	2.44193900	-1.32795800
H	-1.86126500	0.38911100	2.09309100
H	-2.58697500	-1.04475800	1.38327200
H	-0.92644500	-1.08524900	1.94348300
H	-3.22105500	0.19989200	-0.70450300
H	-2.61624400	1.66666600	0.04314800
H	-2.05860300	1.19981500	-1.55463100
H	1.41786400	0.16566300	-1.33659100
H	3.59516600	0.28996300	-0.17353200
H	2.77703100	1.84091500	-0.08598300
H	2.79868100	0.78149900	1.31130400

1a-a-TS2

C	0.13357500	2.27211000	-0.21511800
C	0.25055100	0.92064600	0.28892800
C	1.44863200	0.12352000	-0.25464300
C	2.77148600	0.75326300	0.19262800
C	1.38313200	-1.34647900	0.18188800
C	0.18325200	-2.10204900	-0.43475400
C	-0.91317900	-1.14941700	-0.83593500
C	-1.27457600	-0.03423400	0.02673100
C	-2.35493300	0.84084800	-0.60938100
C	-1.70577400	-0.45672600	1.43714100
H	-1.05528500	-1.00545600	-1.89579700
H	0.29264200	0.93100500	1.37239900
H	-0.18235700	-2.84908600	0.26676000
H	0.51023200	-2.64965300	-1.31311000
H	1.33578100	-1.37923000	1.26836200
H	2.30596400	-1.84972500	-0.09194400
H	-0.44036100	3.00703500	0.31982600
H	0.34625400	2.49323200	-1.24762000
H	-1.86584400	0.41287300	2.06766400
H	-2.63894000	-1.01133900	1.39423300
H	-0.96933100	-1.08572900	1.92360300
H	-3.26336100	0.25964100	-0.74609300
H	-2.59978700	1.69527700	0.01186900
H	-2.04887300	1.21050600	-1.58214800
H	1.41270400	0.15898500	-1.34404000
H	3.61803100	0.20710300	-0.21413900
H	2.85001900	1.78524700	-0.13127000
H	2.85951800	0.74041900	1.27653200

1b-g-path: gauche 1 → (+)-4

1b-g-TS1

C	1.41256100	-0.22056900	-0.19829900
C	-1.22731500	-1.74992800	-0.13253000
C	-2.14267500	-0.73521300	-0.75779900
C	-1.49029200	0.64957900	-0.85791700
C	-0.78629100	1.04200400	0.44740800
C	0.29978800	-0.00556900	0.82324300
C	-0.46994300	-1.34132800	1.10015200
C	2.24601400	0.97355900	-0.61353100
C	2.16340000	-1.53273900	-0.23081700
C	-0.34798500	2.51054100	0.44129200
H	-1.48015600	-2.79115200	-0.25453500
H	0.75822900	0.32465200	1.76137900
H	-2.46770600	-1.07113900	-1.73878200
H	-3.04846700	-0.65165200	-0.15023800
H	-0.76937300	0.65279000	-1.67148400
H	-2.24701000	1.39037800	-1.10560300
H	0.20459300	-2.12395300	1.42445300
H	-1.15945200	-1.17426100	1.93071800
H	2.45582000	1.63413400	0.22580400
H	3.19941700	0.65834600	-1.02367400
H	1.75604100	1.57144000	-1.37531900
H	2.77563400	-1.58762300	-1.12538100
H	2.84038800	-1.62176600	0.62235900
H	1.51793700	-2.39911900	-0.23074600
H	-1.52664900	0.96698200	1.24431900
H	-1.22571600	3.15078000	0.45251900
H	0.24264400	2.75169400	1.32060500
H	0.23026100	2.77745500	-0.43360300

1b-g-IM

C	-1.56935600	0.06170400	0.17740900
C	-0.40507300	0.06057600	-0.76597400
C	0.21919800	-1.42593200	-0.98108300
C	1.23451700	-1.79025600	0.03738500
C	0.76000300	1.05180900	-0.50571300
C	1.76961200	0.59492400	0.55983500
C	2.34234200	-0.79935600	0.25466100
C	-2.90667900	-0.34453200	-0.38962600
C	-1.37931400	-0.18977300	1.64887700
C	0.26008600	2.47357100	-0.23908000
H	2.58135500	1.31796400	0.60233500
H	1.31297300	0.59066700	1.54451100
H	3.00235700	-1.11817700	1.05560900
H	1.09004500	3.17429600	-0.21339000
H	2.95187500	-0.73439200	-0.64741500
H	-0.85673800	-1.13247700	1.82385600
H	-0.26284300	2.54573900	0.70893900
H	1.31541200	1.08342800	-1.44447000
H	-2.33416300	-0.24679000	2.16126900
H	-0.42464000	2.79893800	-1.01696000
H	0.69102400	-1.39101300	-1.96136500
H	0.95942000	-2.44259100	0.84893300
H	-0.79756600	0.58618500	2.13318600
H	-0.80731600	0.32891900	-1.73942900
H	-0.58494900	-2.15133500	-1.03602800
H	-3.03849900	-1.42845400	-0.38063800
H	-3.72016600	0.07454300	0.19610300
H	-3.02959300	-0.01186000	-1.41519100

1b-g-TS2

C	-1.59031900	0.09146100	0.14289100
C	-0.45641000	0.10464400	-0.75276600
C	0.26492500	-1.56249000	-0.92030000
C	1.21527100	-1.81453600	0.12377600
C	0.76173200	1.03181300	-0.52972400
C	1.76538800	0.57976000	0.54541900
C	2.33533400	-0.82313800	0.27244100
C	-2.90624500	-0.42083200	-0.38836700
C	-1.41481800	-0.00668500	1.63309400
C	0.32972600	2.48698500	-0.31829400
H	2.58160200	1.29851400	0.57225600
H	1.30912500	0.59956600	1.53030100
H	3.01215200	-1.11144200	1.07115200
H	1.19140500	3.14893800	-0.32449500
H	2.92359300	-0.79055800	-0.64429100
H	-0.87545100	-0.92098300	1.89424700
H	-0.18400200	2.62111400	0.62778500
H	1.31016300	1.00414300	-1.47189200
H	-2.37370800	-0.03728200	2.13998500
H	-0.34421100	2.81049100	-1.10583700
H	0.72317300	-1.43439100	-1.89294900
H	0.89040900	-2.33609100	1.01023100
H	-0.85222500	0.82091900	2.04838200
H	-0.80855700	0.25645400	-1.76624200
H	-0.56048600	-2.25745700	-0.97903500
H	-3.04599200	-1.47910300	-0.16082400
H	-3.73970600	0.10880600	0.06611100
H	-2.98479100	-0.30353400	-1.46391700

1b-a-path: anti 1 → (+)-4

1b-a-TS1

C	1.05066200	1.52824100	-1.33911400
C	-0.27610300	-0.93824600	-0.59660700
C	-1.54236600	-0.11017100	-0.50538700
C	-1.49702600	0.83553800	0.70601900
C	-0.17811800	1.62931000	0.85681300
C	1.02675900	1.04057800	0.08928500
C	1.00272700	-0.53778100	0.10904700
C	2.21262100	-1.12238900	-0.64007800
C	1.06460100	-1.07966700	1.55382900
C	-2.79052300	-0.99697800	-0.45621000
H	-2.33511200	1.52501300	0.65223300
H	-1.66250600	0.24032500	1.59966100
H	0.06728400	1.69725900	1.91191000
H	-3.69524700	-0.39632100	-0.42287700
H	-0.32253000	2.65292000	0.52447400
H	0.25589900	-0.71839900	2.17586200
H	-2.78126800	-1.63742900	0.42200100
H	-1.62162200	0.49863400	-1.40460200
H	2.00062600	-0.79753900	2.02974900
H	-2.84900300	-1.63556400	-1.33286100
H	0.48903300	2.40397000	-1.61285900
H	1.93832600	1.37424000	0.58928500
H	1.01249300	-2.16458700	1.54925400
H	-0.37288900	-1.96934400	-0.90068400
H	1.87788700	1.28234400	-1.97822000
H	3.14570500	-0.75668100	-0.21843400
H	2.21639200	-2.20538900	-0.55371000
H	2.19712700	-0.88406100	-1.69576800

1b-a-IM

C	1.14828900	0.81849900	0.38933400
C	0.70834300	-0.73427500	0.01844900
C	0.48077300	-1.46961600	1.35581500
C	2.47978900	1.22663400	-0.13872100
C	-0.54499000	-0.74603700	-0.80890600
C	-1.73354800	0.14897100	-0.54992300
C	-1.34097200	1.33307100	0.34491000
C	0.05988200	1.82463300	-0.01276700
C	1.80986400	-1.47807700	-0.75210800
C	-2.95202200	-0.61448900	-0.01254300
H	-2.06794300	2.13219100	0.22644200
H	-1.37019400	1.04789500	1.39486500
H	0.26894100	2.77399700	0.47276900
H	-3.80154300	0.05274900	0.10973000
H	0.10829500	2.01028400	-1.08526700
H	-0.30051400	-1.00475000	1.94677300
H	-2.73976600	-1.06619800	0.95174300
H	-2.02442500	0.56936700	-1.51342500
H	1.38988200	-1.46884500	1.95205600
H	-3.24668400	-1.40791600	-0.69278900
H	2.57397500	1.59123600	-1.14727500
H	1.21275100	0.83253100	1.47400500
H	0.19484600	-2.50256400	1.18156200
H	-0.51866600	-1.26023500	-1.75516700
H	3.38204500	0.87572400	0.32903200
H	2.72786900	-1.54840100	-0.17899700
H	1.48076900	-2.49009800	-0.97181500
H	2.03791300	-0.99284800	-1.69548600

1b-a-TS2

C	1.18996500	0.87805800	0.41065200
C	0.64213000	-0.81807300	-0.01631000
C	1.77751700	-1.58728000	-0.69379600
C	2.50924000	1.18119000	-0.09049200
C	0.09368300	1.85772400	-0.01508500
C	-1.31449100	1.35991600	0.31965700
C	-1.71738200	0.16827000	-0.56953300
C	-0.50405900	-0.67876600	-0.90419200
C	-2.89367400	-0.62737900	0.01082200
C	0.33328200	-1.45268600	1.34667500
H	-2.03486800	2.16292000	0.18735900
H	-1.35821400	1.08809800	1.37205600
H	0.27460000	2.81100500	0.47495400
H	-3.74808500	0.02324100	0.17981200
H	0.16556700	2.04565900	-1.08543000
H	-0.44262300	-0.92691300	1.88797500
H	-2.63732900	-1.09106200	0.95754300
H	-2.06228700	0.58874700	-1.51255900
H	1.22142400	-1.46257300	1.97169200
H	-3.20354600	-1.41423800	-0.67002300
H	2.64433100	1.56150900	-1.08889800
H	1.20925300	0.79933600	1.49063200
H	0.00881700	-2.48118900	1.21648600
H	-0.30020100	-0.79116300	-1.95799200
H	3.38279700	0.77562000	0.38726200
H	2.65288200	-1.65436700	-0.05721700
H	1.45358300	-2.60054100	-0.91827000
H	2.07663600	-1.11992700	-1.62576700

2a-g-path: gauche 2 → (+)-3

2a-g-TS1

C	0.21983000	-1.29665500	0.81061300
C	0.91395900	-1.20304300	-0.52191000
C	1.79387900	-0.00312300	-0.78099800
C	1.06230000	1.29695200	-0.39576200
C	0.28191500	1.19176200	0.92111100
C	-0.66510300	-0.02283400	0.94990000
C	-1.69858900	-0.00814500	-0.16969400
C	-2.44845300	1.27914100	-0.42179800
C	3.15152100	-0.13937100	-0.06684500
C	-2.54441500	-1.24054500	-0.39262200
H	-1.17928300	-0.02815500	1.91651900
H	1.18586800	-2.12021500	-1.02180500
H	-0.26601500	2.11297800	1.09245000
H	0.97244800	1.09956800	1.75660600
H	0.37152600	1.54537600	-1.19501100
H	1.77392200	2.11720300	-0.33509200
H	-0.37207900	-2.20043100	0.88045000
H	0.93533400	-1.33957800	1.63397100
H	-3.03065800	1.21455100	-1.33554700
H	-3.14947600	1.48082500	0.39134800
H	-1.79981500	2.14155900	-0.50643500
H	-3.25145000	-1.37827400	0.42878300
H	-3.12958800	-1.13957900	-1.30116300
H	-1.96571800	-2.14956400	-0.48038600
H	2.00367100	0.03782400	-1.84781800
H	3.80499100	0.68860200	-0.32705100
H	3.04414100	-0.14781100	1.01331200
H	3.65112100	-1.05972100	-0.35510000

2a-g-IM

C	-0.33123500	0.78833700	-1.23030100
C	0.69422300	-0.28672000	-0.80354100
C	-0.07184500	-1.41219400	0.08857900
C	-0.98692800	-0.83204800	1.10395800
C	-2.01058800	0.17263900	0.62903800
C	-1.27901500	1.29842400	-0.13272700
C	1.96478400	0.19842700	-0.17946200
C	3.14096300	-0.74414300	-0.19261400
C	-3.12769300	-0.47243500	-0.20484400
C	1.94750800	1.21852400	0.92513600
H	0.98752400	-0.81604900	-1.70616000
H	-0.63154000	-0.73675100	2.11725300
H	0.19372300	1.63194900	-1.67043300
H	-0.93278800	0.36485000	-2.03116500
H	-0.72666100	1.89234300	0.58743600
H	-2.00758300	1.96876100	-0.58428400
H	0.65893700	-2.07518700	0.53763200
H	-0.63880600	-2.00129400	-0.62753800
H	1.38658400	0.85819500	1.79075400
H	2.95394400	1.44492400	1.26221800
H	1.48974400	2.15170800	0.61490500
H	4.07861700	-0.19497100	-0.18105900
H	3.14821600	-1.39654300	0.68267300
H	3.13889300	-1.38103100	-1.07153800
H	-2.48450600	0.62040200	1.49914500
H	-3.86026600	0.27294200	-0.50193100
H	-2.75337600	-0.94163200	-1.10844000
H	-3.64169700	-1.23548600	0.37120100

2a-g-TS2

C	-0.15219100	-1.46718200	0.11081600
C	-1.01534000	-0.86862200	1.09022600
C	-2.03292100	0.14687400	0.62284500
C	-1.27241300	1.30426400	-0.05961300
C	-3.12505300	-0.45524400	-0.27159500
C	-0.31419100	0.86467600	-1.17993100
C	0.74789600	-0.19796300	-0.83228600
C	1.97906900	0.18732500	-0.18264400
C	1.98235700	1.17808600	0.94736800
C	3.14251200	-0.77007300	-0.22672000
H	-2.53238500	0.55931500	1.49628800
H	0.97843900	-0.77326700	-1.72016700
H	-0.63123100	-0.73766200	2.09028600
H	0.18369200	1.74585700	-1.57616400
H	-0.90814900	0.47147400	-2.00095700
H	-0.72342000	1.84635800	0.70338200
H	-1.98585400	2.01057500	-0.47975900
H	0.58991600	-2.14474900	0.50818000
H	-0.67928800	-1.93301300	-0.71041700
H	1.40839000	0.79897800	1.79718600
H	2.99084100	1.37381000	1.29677200
H	1.54232400	2.12838000	0.66408100
H	4.08648400	-0.23272700	-0.26965700
H	3.17956700	-1.39861700	0.66479200
H	3.09414200	-1.42751100	-1.08855000
H	-3.84832700	0.30514000	-0.55305400
H	-2.72800800	-0.88178800	-1.18636100
H	-3.65548700	-1.24340500	0.25332900

2a-a-path: anti 2 → (+)-3

2a-a-TS1

C	0.99875200	1.08815400	-0.78701400
C	-0.29107100	-1.44917400	-1.29596100
C	-0.38234200	1.65434100	-1.01274800
C	-1.37672800	1.31200700	0.11254100
C	-1.30720300	-0.14612600	0.65123000
C	-0.09288300	-0.93979100	0.11091700
C	1.22497300	-0.05970600	0.17295000
C	-2.63051900	-0.89519400	0.46010100
C	2.44292900	-0.88720100	-0.26854200
C	1.51430500	0.45169000	1.60073800
H	-1.16017700	-0.07990000	1.72452400
H	1.84638300	1.70854900	-1.03213900
H	0.05116300	-1.79765600	0.76806200
H	-0.32723900	2.73591400	-1.10917300
H	-0.77198000	1.30078500	-1.96498100
H	-1.19850000	1.99544500	0.93741700
H	-2.38253800	1.52967800	-0.23573000
H	0.23323800	-2.32170200	-1.63653600
H	-1.05415500	-1.06017600	-1.94023500
H	1.61408800	-0.37666300	2.29827900
H	2.44864800	1.00559200	1.61308100
H	0.74371600	1.11327400	1.97636000
H	3.34559700	-0.28427800	-0.22106500
H	2.58648900	-1.74458500	0.38484300
H	2.34340400	-1.24527400	-1.28521300
H	-3.42707500	-0.39471800	1.00350400
H	-2.92941700	-0.94547800	-0.58156100
H	-2.56292400	-1.91280300	0.83529000

2a-a-IM

C	-1.36521300	0.63897400	-0.44915700
C	0.16550000	0.76922500	-0.68673300
C	1.07469000	-0.31136800	0.08306700
C	0.42811000	-1.66860100	-0.05593600
C	-1.05398700	-1.83514000	0.11417900
C	-1.81975100	-0.80332500	-0.71986300
C	0.65391800	2.18138200	-0.52855200
C	1.28721700	0.02655300	1.57253100
C	2.45671700	-0.35031200	-0.59233000
C	-1.90988600	1.16073200	0.88825500
H	-1.81928000	1.26427000	-1.21562000
H	1.05938600	-2.52989800	0.09436800
H	0.29786000	0.50977600	-1.73503700
H	-1.34862500	-2.83786900	-0.18307200
H	-1.33224100	-1.74351600	1.16589600
H	-1.66276800	-1.02843200	-1.77272100
H	-2.88804500	-0.89372000	-0.53816400
H	1.37566100	2.58183600	-1.21647700
H	0.52702700	2.71489300	0.39486100
H	2.97345300	0.59932700	-0.49897100
H	3.08215800	-1.11001700	-0.13166400
H	2.37281800	-0.58820300	-1.64842300
H	1.95028900	-0.70671100	2.02295400
H	1.74858600	1.00198300	1.69222400
H	0.36657100	0.02099200	2.14054200
H	-2.99544200	1.17943500	0.85006300
H	-1.63176200	0.54441000	1.73371900
H	-1.57953900	2.17272800	1.09276400

2a-a-TS2

C	0.43696000	2.27104100	-0.44118600
C	0.06100500	0.90053800	-0.71912800
C	-1.42129500	0.52642300	-0.51085000
C	-1.61901700	-0.98715000	-0.68923700
C	-0.91853700	-1.83449300	0.39590800
C	0.27680800	-1.12036700	0.97464900
C	1.13348300	-0.28624900	0.14235900
C	1.81900700	-1.05864500	-0.99356000
C	-2.04151900	1.05010600	0.79016800
C	2.18431000	0.44110500	0.98298500
H	0.22548300	-0.87319300	2.02279400
H	0.31533200	0.66538900	-1.74519600
H	-0.63600400	-2.79885800	-0.02307600
H	-1.61600400	-2.05282500	1.19848900
H	-1.24408000	-1.26178100	-1.67182300
H	-2.68107600	-1.21647600	-0.69991900
H	1.31178900	2.68682300	-0.90857000
H	0.08170700	2.78861800	0.43121600
H	2.36129900	-0.38304000	-1.64866300
H	2.53244700	-1.76892300	-0.58536000
H	1.11238200	-1.61272300	-1.60065000
H	2.82182200	-0.28575100	1.48008800
H	2.81930500	1.07617500	0.37558600
H	1.72660800	1.05888300	1.74827400
H	-1.96342200	1.00528900	-1.32441800
H	-3.05694800	0.67901700	0.89751600
H	-1.48487400	0.74618500	1.67008300
H	-2.09299000	2.13333700	0.79098000

2b-g-path: gauche 2 → (-)-4

2b-g-TS1

C	-0.70468700	-1.10783200	0.07858300
C	-1.25480200	-0.30824400	1.27141000
C	-1.86655600	1.03935300	0.86777400
C	-0.95441600	1.81207300	-0.04231400
C	-0.29972400	1.07877500	-1.17818100
C	0.33983000	-0.27171600	-0.70824400
C	1.61995600	-0.09124000	0.09077700
C	2.37374200	-1.34933400	0.46175700
C	-1.81901300	-1.65612600	-0.82206300
C	2.44109700	1.17141700	0.04104500
H	-1.99349300	-0.90407700	1.80238000
H	-0.44256300	-0.12324300	1.96900400
H	-2.09139100	1.62180200	1.75735000
H	-2.82502700	0.87426400	0.37027400
H	2.17687800	-1.65171800	1.48941500
H	-0.19135200	-1.97447500	0.48598500
H	3.44728000	-1.20605800	0.37538000
H	-1.03867800	0.85598700	-1.94959200
H	-1.14558200	2.86597300	-0.16749900
H	2.10509200	-2.18940800	-0.17359400
H	0.59455000	-0.83704500	-1.60958400
H	0.44819200	1.69886200	-1.65992200
H	3.13296800	1.19818400	0.87820800
H	3.04493800	1.22298200	-0.86802500
H	1.83951200	2.06897100	0.08925600
H	-2.48381100	-2.29980500	-0.25286100
H	-2.42682000	-0.87586400	-1.26675800
H	-1.40325100	-2.24808300	-1.63267800

2b-g-IM

C	2.02078600	-1.23157400	-0.02455200
C	0.82147900	-1.67159700	-0.81499200
C	0.03684100	-0.58357500	-1.44819700
C	-0.40712500	0.58559000	-0.40313200
C	0.78744800	0.97061600	0.51656000
C	1.58653300	-0.23301600	1.06139200
C	-1.70382600	0.28456000	0.28342800
C	-1.76535100	-0.66225000	1.45009500
C	1.71458700	1.96732700	-0.19574500
C	-2.96103900	0.39830100	-0.54067500
H	2.45941200	0.13852100	1.59324100
H	0.99102400	-0.76798700	1.79354500
H	2.52136100	-2.07857700	0.43480100
H	2.74637600	-0.76359200	-0.68793200
H	-1.42558200	-1.66194000	1.16932100
H	0.37564800	1.49459500	1.37610100
H	-2.78105200	-0.75752300	1.82035300
H	0.65108100	-0.08748300	-2.19574800
H	0.31269400	-2.57019700	-0.50500000
H	-1.14580000	-0.33610800	2.27844500
H	-0.60350700	1.44372800	-1.03987300
H	-0.84532300	-0.95553400	-1.95658900
H	-3.20075100	-0.53829300	-1.04764300
H	-3.81464100	0.64161000	0.08631500
H	-2.87744800	1.16710100	-1.30227600
H	2.53748700	2.25902500	0.45032600
H	2.14280900	1.55720800	-1.10500200
H	1.17421100	2.86914600	-0.46747500

2b-g-TS2

C	0.09466100	-0.82882600	-1.42113200
C	0.87444000	-1.75181100	-0.64684700
C	2.07061500	-1.18067000	0.06168200
C	1.59571400	-0.11899000	1.06740300
C	0.76176400	1.02508300	0.44866600
C	1.65250400	1.98296200	-0.35678700
C	-0.45600600	0.58146500	-0.40572600
C	-1.71810800	0.29955300	0.24032800
C	-1.77615200	-0.49882200	1.51220600
C	-2.96846900	0.29044600	-0.60167700
H	2.45241800	0.31958900	1.57407500
H	1.01371200	-0.61888000	1.83537400
H	2.62581200	-1.95414000	0.58406100
H	2.75506000	-0.73535500	-0.65748000
H	-1.40866300	-1.51546400	1.34841900
H	0.36980100	1.60315300	1.28235200
H	-2.79322500	-0.57628700	1.88237200
H	0.68016000	-0.29239700	-2.15603900
H	0.37395700	-2.58293100	-0.17352600
H	-1.17125500	-0.06492100	2.30130500
H	-0.61813500	1.30141800	-1.19793100
H	-0.79488800	-1.23776000	-1.87820500
H	-3.21982100	-0.71699500	-0.93792300
H	-3.82163900	0.65184800	-0.03319100
H	-2.86797900	0.91412300	-1.48386400
H	2.49041900	2.32758100	0.24192100
H	2.05787500	1.51758600	-1.24974100
H	1.09060900	2.85749800	-0.67067000

2b-a-path: *anti* 2 → (-)-4

2b-a-TS1

C	1.03880500	-0.46070300	0.00191500
C	-0.20567100	-1.09320800	-0.57850600
C	-1.59145900	-0.82618500	-0.04474000
C	-1.54062500	0.13941500	1.14782500
C	-0.65663900	1.36349000	0.88993400
C	0.76388400	1.08509400	0.30548700
C	-2.52025400	-0.32798500	-1.16416700
C	0.99368700	1.97895400	-0.88813800
C	2.19480300	-0.64701200	-0.99567100
C	1.46989200	-1.16527000	1.31053900
H	-2.54560100	0.47947700	1.38578300
H	-1.19527300	-0.39542300	2.02525800
H	-0.56258300	1.92914100	1.81254700
H	-1.18657400	2.01368100	0.20180200
H	0.76950200	-1.01752900	2.12191200
H	-2.01107300	-1.76753900	0.31273400
H	2.43520600	-0.78995200	1.64061900
H	0.51472100	2.94290500	-0.89956000
H	1.49978600	1.36540900	1.06125400
H	1.56874800	-2.23497500	1.15029300
H	-0.07404500	-1.97418100	-1.18700500
H	1.90620200	1.91132700	-1.45055000
H	3.09064100	-0.12711700	-0.66689900
H	2.44129100	-1.70177600	-1.07780100
H	1.93771200	-0.29344200	-1.98662200
H	-3.53472700	-0.19637300	-0.79718500
H	-2.18028000	0.61874200	-1.57159100
H	-2.55218800	-1.04191300	-1.98186300

2b-a-IM

C	0.04671400	1.72784700	0.29620600
C	-0.95804100	0.83678000	-0.44499900
C	-0.80479800	-0.71548600	0.07091600
C	0.62980100	-0.91027400	0.47351900
C	1.68477200	-0.16304900	-0.29511700
C	1.50757300	1.35243700	-0.01823200
C	-2.35032300	1.34275200	-0.34493500
C	-1.18554600	-1.63998500	-1.09605300
C	-1.71958700	-1.01340400	1.26772300
C	3.10169000	-0.64107000	0.01942200
H	1.51042500	-0.32741200	-1.35666200
H	2.13829300	1.64289400	0.81818600
H	1.86012800	1.91657800	-0.87847100
H	-0.12832500	2.76885400	0.04136800
H	-0.13446700	1.64356800	1.36583400
H	-0.50607400	-1.52802700	-1.93486200
H	-2.18979800	-1.42120000	-1.44966100
H	-2.70298800	1.76758100	0.57919600
H	-0.68126000	0.81516100	-1.49668200
H	-1.16055300	-2.68042100	-0.78645600
H	0.83353300	-1.06434500	1.52406100
H	-3.10500100	0.99009000	-1.02574200
H	-2.76838500	-0.98530100	0.99451500
H	-1.50491500	-2.00633000	1.65300600
H	-1.56462800	-0.30658800	2.07779100
H	3.83930300	-0.06309400	-0.53043200
H	3.32104700	-0.53502000	1.07884200
H	3.23014400	-1.68628400	-0.24452900

2b-a-TS2

C	1.88530600	-1.31542900	-0.92640800
C	0.83008000	-0.75876900	0.02976000
C	1.02353100	-1.34874600	1.43169100
C	-0.51375700	-0.92260700	-0.50647000
C	-1.72260700	-0.38512600	0.22423900
C	-2.97530600	-0.49507500	-0.64885000
C	-1.45586100	1.08142200	0.66849500
C	-0.26996800	1.71976600	-0.06162400
C	1.05612600	1.02963800	0.26247300
C	2.20520600	1.54141300	-0.44946000
H	-2.34748700	1.68033100	0.50500800
H	-1.26091400	1.11933900	1.73780000
H	-0.19702300	2.76700100	0.22077500
H	-0.43936800	1.70396800	-1.13681000
H	0.29167500	-0.97633800	2.13963600
H	-1.89545300	-0.98580800	1.11492300
H	2.00908400	-1.10510500	1.81752900
H	2.12323200	1.84657200	-1.47895100
H	1.23245000	1.06855300	1.33076700
H	0.93705200	-2.43133000	1.40218800
H	-0.59739100	-0.95461100	-1.58321000
H	3.19989800	1.35506200	-0.08589500
H	2.89071400	-1.15896700	-0.55163900
H	1.74069100	-2.38554300	-1.05165900
H	1.81813400	-0.85515000	-1.90651900
H	-3.13484600	-1.51871100	-0.97502100
H	-3.85923100	-0.17504200	-0.10539800
H	-2.88771300	0.12685200	-1.53659200

1a-concerted path: 1 → (-)-3

1a-concD0, second order saddle point

C	0.62516900	0.01932200	1.45062600
C	-1.10329400	-0.28746400	-0.04338400
C	-1.26921700	1.14144900	-0.14481900
C	0.45925200	1.44818700	1.34919500
C	-0.15502400	1.55096700	-1.14514800
C	1.20114800	0.67310000	-1.00901100
C	1.58785300	-0.25397700	0.26886200
C	-2.02438800	-0.93858200	0.99475500
C	-1.16667200	-1.12929400	-1.31758700
C	1.82726700	-1.72423400	-0.07477000
H	-2.16442100	1.70408200	0.03751400
H	0.45703800	-0.60501500	2.30287300
H	-0.50087400	1.42640000	-2.17147500
H	0.10156400	2.60016900	-1.05046700
H	1.27663000	0.04272700	-1.88508000
H	2.01282300	1.38486700	-1.12174800
H	-0.01537300	1.98806800	2.15655500
H	1.14733500	2.03946500	0.79014800
H	-1.07784300	-2.18411800	-1.08638100
H	-2.15480900	-0.98865900	-1.75562700
H	-0.44482800	-0.89541100	-2.08141300
H	-3.03473100	-1.04810100	0.59702000
H	-1.68319500	-1.93152000	1.27472700
H	-2.09409800	-0.34304400	1.89881900
H	2.56505300	0.12051200	0.57779100
H	2.53127600	-1.82263300	-0.89655100
H	2.26109000	-2.23082000	0.78390700
H	0.92480700	-2.25381700	-0.34292100