Supporting Information

DFT CALCULATIONS

General considerations: The DFT calculations were carried at the B3LYP/6-311g** level of theory, unless otherwise stated, using the program package Gaussian09.[1] Optimized structures were identified as energy minima by calculating the vibrational frequencies. E is the absolute electronic energy with zero point energy correction; H and G are the sum of electronic(in hartrees). Transition states were examined by vibrational analysis and then submitted to intrinsic reaction coordinate calculations.

[1] *Gaussian 09, Revision 4.2.0*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N.; Staroverov, R. Kobayashi, J. Normand, K., Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, ***2009***.

Cartesians coordinates for the optimized structure of (1*E*-3*Z*)-4
(E = -1130.533263; H = -1130.514037; G = -1130.580359)

atom	x	y	z
C	-4.49120500	-1.17238400	0.10249700
C	-3.83176800	-1.49078800	-1.08505400
C	-2.50126800	-1.13530500	-1.27274600
C	-1.79445000	-0.42583100	-0.28488400
C	-2.46886500	-0.11651600	0.91287900
C	-3.79632400	-0.49053600	1.09995200
H	-5.52579700	-1.45898800	0.25129700
H	-4.35569800	-2.02936400	-1.86773700
H	-1.97780700	-1.39864100	-2.18474700
H	-1.93857900	0.41127400	1.69769100
H	-4.29063600	-0.24793300	2.03509000
N	-0.43253100	-0.18515200	-0.48122700
C	0.18756200	0.91560800	-0.19185400
C	1.65893900	0.93014200	-0.18178100
C	2.47289100	-0.13997400	-0.02863500
N	-0.40651400	2.15621700	0.00934500
N	2.25950100	-1.34492600	0.54709800
Cl	4.18558700	0.12085500	-0.55907200
H	2.13742700	1.86652300	-0.43073400
C	-1.64932000	2.53812100	-0.64474800
H	-1.51958400	3.52531700	-1.10312100
H	-1.90006400	1.82648400	-1.42734900
H	-2.49243800	2.58674100	0.05416400
C	0.24714800	3.22849300	0.74359300
H	-0.47852000	3.70512200	1.41226400
H	1.05748900	2.83669600	1.35508600
H	0.64985900	4.00540200	0.07817400
C	1.26055800	-1.50358200	1.59693000
H	0.28811800	-1.79829200	1.19549400
H	1.61911600	-2.26721400	2.29355800
H	1.14627300	-0.56245000	2.13398700
C	2.70847100	-2.58855100	-0.07191500
H	1.88788700	-3.05494900	-0.63000800
H	3.53273300	-2.39538400	-0.75350400
H	3.04784300	-3.28122600	0.70269100

Cartesians coordinates for the optimized structure of (1*Z*-3*Z*)-4
(E = -1130.530154; H = -1130.510858; G = -1130.578189)

atom	x	y	z
C	4.67006000	-1.10929100	-0.16121100
C	4.15947000	-1.19923300	1.13435600
C	2.83411800	-0.87427500	1.39714900
C	1.98438000	-0.42233600	0.37155300
C	2.50669200	-0.34572100	-0.93407200
C	3.83055800	-0.68925800	-1.19150200
H	5.70067000	-1.37534800	-0.36588200
H	4.79666100	-1.53707500	1.94501300
H	2.42544200	-0.96708900	2.39684000
H	1.85518300	-0.03849200	-1.74462000
H	4.20712500	-0.63197700	-2.20771200
N	0.63848200	-0.20203000	0.65472800
C	-0.06824200	0.79935000	0.25736100
C	-1.54042300	0.70146300	0.33847600
C	-2.31189400	-0.36430700	0.03333000
N	0.40290000	2.04536000	-0.14156800
N	-3.63040400	-0.52162400	0.39324800
H	-2.05304900	1.57671600	0.72003600
C	1.71359200	2.54331100	0.24156500
H	1.62746800	3.61113900	0.47097200
H	2.06759600	2.02621900	1.13048100
H	2.46501300	2.41623800	-0.54735700
C	-0.32584300	2.89686900	-1.06844000
H	0.27407200	3.08035800	-1.96976700
H	-1.25273000	2.41657000	-1.37430700
H	-0.56119000	3.87032700	-0.61875300
C	-4.17986300	0.39652000	1.38024200
H	-4.41063000	1.38808100	0.96146700
H	-5.10587700	-0.02932700	1.77137200
H	-3.47474700	0.51882800	2.20259800
C	-4.61501700	-1.05297100	-0.54727100
H	-5.02108000	-0.26531700	-1.19870900
H	-4.16617300	-1.82279800	-1.16847300
H	-5.43900300	-1.49766300	0.01442800
Cl	-1.63277200	-1.74541600	-0.83951200

Cartesians coordinates for the optimized structure of (1*Z*-3*E*)-4
(E = -1130.538214; H = -1130.518897; G = -1130.586185)

atom	x	y	z
C	-4.02576400	0.47952100	0.15381000
C	-3.59706600	-0.07424100	-1.05244500
C	-2.40518300	-0.78652700	-1.12028400
C	-1.59718900	-0.94511800	0.01680100
C	-2.04364400	-0.39468300	1.23054900
C	-3.24472000	0.30662400	1.29479300
H	-4.96082600	1.02539900	0.20611100
H	-4.19960800	0.04340700	-1.94692400
H	-2.07539700	-1.23202400	-2.05128300
H	-1.45531200	-0.55025300	2.12792000
H	-3.57524700	0.71330700	2.24513000
N	-0.44833700	-1.73601200	-0.07656000
C	0.72064500	-1.34435500	0.29631800
C	1.08452400	0.04646500	0.68960000
C	1.05929000	1.13264700	-0.10101100
N	1.72366500	-2.28594100	0.42498100
N	1.11792000	2.44481300	0.30822400
H	1.36842600	0.19149700	1.72627900
C	1.39612800	-3.67873600	0.15430200
H	2.15077800	-4.31472200	0.62360700
H	0.41314000	-3.90744300	0.55984700
H	1.37154700	-3.89308000	-0.92260600
C	3.12785000	-1.94196000	0.25404300
H	3.46646300	-2.12478300	-0.77582700
H	3.29002400	-0.89113500	0.48303900
H	3.74178100	-2.54710700	0.92749800
C	0.90404600	2.71529800	1.72281300
H	1.78059000	2.47343600	2.34412100
H	0.68746700	3.77862600	1.84330400
H	0.04845000	2.14079700	2.07770700
C	2.00307600	3.39328900	-0.36380200
H	3.03069600	3.33986200	0.02537300
H	2.02405900	3.19582900	-1.43261200
H	1.62502500	4.40568700	-0.20749900
Cl	0.83666200	0.92608000	-1.85309600

Cartesians coordinates for the optimized structure of (1*E*-3*E*)-4
(E = -1130.540022; H = -1130.520624; G = -1130.587279)

atom	x	y	z
C	3.62907200	-1.31108400	-0.50374100
C	3.08843000	-1.76370300	0.69927300
C	1.70966800	-1.81900700	0.87671300
C	0.82911000	-1.40062400	-0.13703100
C	1.38742000	-0.96868700	-1.35530200
C	2.76664900	-0.92557500	-1.52979800
H	4.70294800	-1.27856000	-0.64726900
H	3.74352800	-2.09119500	1.49984600
H	1.28598400	-2.20467700	1.79711800
H	0.73080400	-0.68190300	-2.16740700
H	3.17093800	-0.59334300	-2.48029800
N	-0.54117300	-1.54999600	0.07822400
C	-1.44264400	-0.68227800	-0.25521900
C	-1.21150200	0.72063000	-0.67405400
C	-0.35287100	1.58763900	-0.09956900
N	-2.75764500	-1.10610400	-0.30102000
N	0.20529000	1.56046800	1.13631100
H	-1.74379300	1.05559800	-1.55442100
C	-3.04743700	-2.51245100	-0.06180200
H	-4.01333300	-2.75378800	-0.51288000
H	-2.26666800	-3.12636600	-0.50412600
H	-3.09123800	-2.74644100	1.01068300
C	-3.87726300	-0.20507700	-0.07172800
H	-4.25180800	-0.28695300	0.95931300
H	-3.58122400	0.82722300	-0.24300300
H	-4.70081700	-0.44970900	-0.74928000
C	-0.47271500	0.88391500	2.23477600
H	-0.19141000	-0.17044000	2.32056800
H	-0.21502900	1.39793600	3.16481400
H	-1.55126700	0.94497000	2.08694300
C	1.58903200	1.95660500	1.39206100
H	2.21052500	1.07556700	1.58093100
H	1.99229700	2.48561000	0.53327100
H	1.62812900	2.61740400	2.26343200
Cl	0.01332000	3.07568700	-1.04943100

Cartesians coordinates for the optimized structure of (1*Z*,2*Z*,3*E*)-4·H$^+$

(E = -1130.941440; H = -1130.922097; G = -1130.989174)

atom	x	y	z	atom	x	y	z
C	-4.22314000	-1.46462000	-0.43632600	H	-0.09268000	-0.69477100	1.17551400
C	-4.30159300	-0.61441600	0.66418900	C	0.39414400	3.58438600	-0.33686600
C	-3.30016000	0.32529600	0.89574600	H	1.23122300	4.11256800	-0.79352100
C	-2.22442200	0.41620600	0.01214300	H	-0.34961300	3.39053700	-1.10896700
C	-2.14820500	-0.42031200	-1.10269600	H	-0.03439800	4.23149700	0.43712100
C	-3.14601400	-1.36620800	-1.31620700	C	2.22854200	2.40845100	0.82062600
H	-5.00324700	-2.19484700	-0.61393500	H	2.26044000	3.27921300	1.48047800
H	-5.13967400	-0.68242300	1.34711300	H	2.43739500	1.51774700	1.40602900
H	-3.35141300	0.98027000	1.75852500	H	2.99102200	2.52212900	0.04780700
H	-1.32618700	-0.32021900	-1.80086200	C	1.61430900	-2.47732500	1.72555300
H	-3.09164500	-2.01364300	-2.18320100	H	0.65102900	-2.97345500	1.56586700
N	-1.23075300	1.42693700	0.23576300	H	2.32706100	-3.21288600	2.09562800
H	-1.58412000	2.35784900	0.40688800	H	1.49679200	-1.69290200	2.47309900
C	0.10611400	1.23759700	0.32840100	C	2.99581300	-2.82322500	-0.29502200
C	0.58220300	-0.08765400	0.58793600	H	3.30463600	-2.36963500	-1.22973700
C	1.67596400	-0.73041600	0.04780800	H	3.88304700	-3.07147200	0.29094100
N	0.89325200	2.32280000	0.22109600	H	2.44478900	-3.74266500	-0.51142100
N	2.14184200	-1.91254100	0.47842000	Cl	2.51728300	-0.01234300	-1.31541300

Cartesians coordinates for the optimized structure of (1*E*,2*E*,3*E*)-4·H$^+$

(E = -1130.936285; H = -1130.917039; G = -1130.982905)

atom	x	y	z	atom	x	y	z
C	3.46081200	-1.65221400	-0.68071400	H	-1.92603200	1.23469400	-1.24207200
C	3.02882500	-2.00814200	0.59434700	C	-3.15564800	-2.39014100	-0.12203900
C	1.68563800	-1.88089900	0.93965200	H	-4.03166000	-2.53995100	-0.75382000
C	0.76719700	-1.40633500	0.00067900	H	-2.32947700	-2.95670400	-0.54996300
C	1.19059300	-1.07255800	-1.28763000	H	-3.38766000	-2.77232700	0.87773700
C	2.53804500	-1.18708800	-1.61668400	C	-3.99836100	-0.05953300	-0.16123000
H	4.50544200	-1.75063500	-0.94911900	H	-4.78610200	-0.45634600	0.48169700
H	3.73415700	-2.38752500	1.32386600	H	-3.72787600	0.93301600	0.19048700
H	1.35158400	-2.16461200	1.93225300	H	-4.38286100	0.00926000	-1.18314200
H	0.47748000	-0.74018400	-2.03082300	C	-0.10348600	1.06355700	2.28477900
H	2.86257000	-0.93130900	-2.61825400	H	0.28755800	0.06582500	2.49203000
N	-0.61486600	-1.35914400	0.37651500	H	0.16094300	1.72606800	3.11057800
H	-0.93185100	-2.15446700	0.91259500	H	-1.18810500	1.02179800	2.20129100
C	-1.57711600	-0.49140400	-0.03899400	C	1.77480500	2.27769500	1.21476300
C	-1.29291200	0.83992400	-0.46122400	H	2.31781600	2.28730600	0.27431300
C	-0.23038900	1.64232400	-0.08270100	H	1.64922500	3.30228900	1.57513000
N	-2.83963700	-0.95731000	-0.09633300	H	2.35068500	1.70779100	1.94314200
N	0.46766600	1.62011500	1.05409900	Cl	0.19847100	2.90525100	-1.22505400

Cartesians coordinates for the optimized structure of (1*Z*,2*E*,3*E*)-4·H$^+$

(E = -1130.939942; H = -1130.920414; G = -1130.987966)

atom	x	y	z	atom	x	y	z
C	-3.97751600	-0.11461700	0.62907900	H	2.09574800	0.30044300	1.17176500
C	-3.71587000	-0.62153400	-0.64132100	C	1.75704000	-3.55240300	0.15874400
C	-2.44351000	-1.08554600	-0.96250200	H	2.52368700	-4.03639500	0.76445200
C	-1.43228200	-1.05250000	-0.00168900	H	0.78963700	-3.72919100	0.62746000
C	-1.69321100	-0.56702200	1.28062300	H	1.77264500	-4.00746400	-0.83749400
C	-2.96413600	-0.08962100	1.58594600	C	3.46963300	-1.76380100	0.08850300
H	-4.96768600	0.24777500	0.87664200	H	3.99405700	-2.45195400	-0.57726100
H	-4.49994100	-0.65316800	-1.38807300	H	3.60299600	-0.75138100	-0.28378800
H	-2.23505200	-1.46618800	-1.95642400	H	3.90428900	-1.84748500	1.08893900
H	-0.91842500	-0.58042000	2.03684600	C	1.44810300	2.68739700	1.71612000
H	-3.16850300	0.28094100	2.58342700	H	2.53845900	2.63631400	1.80670400
N	-0.15663400	-1.60609200	-0.34193300	H	1.11544500	3.65848700	2.08026500
H	-0.19691500	-2.45561700	-0.88758900	H	0.99536200	1.90930000	2.32968800
C	1.07509200	-1.18424300	0.03034100	C	0.88040700	3.81063900	-0.41456900
C	1.36866200	0.17053200	0.38280200	H	0.78398700	3.63398200	-1.47996200
C	0.89070000	1.32404200	-0.21154000	H	0.00074800	4.35293300	-0.05951200
N	2.04539300	-2.11511400	0.10465800	H	1.76963300	4.41931100	-0.23720900
N	1.01738400	2.54607900	0.32094800	Cl	0.10459700	1.23516100	-1.76987200

Cartesians coordinates for the optimized structure of (1*E*,2*Z*,3*E*)-4·H$^+$

(E = -1130.935112; H = -1130.915861; G = -1130.982326)

atom	x	y	z	atom	x	y	z
C	4.44731400	-1.30679800	0.39297900	H	0.29127600	-0.87840100	-1.10848700
C	4.41852800	-0.47718000	-0.72572300	C	-0.56747600	3.40759800	0.22860400
C	3.34687400	0.38867600	-0.92794500	H	-1.45610200	3.91193800	0.60777700
C	2.30873600	0.42633500	0.00314100	H	0.14535500	3.31112300	1.04722700
C	2.33990300	-0.38926400	1.13452600	H	-0.13707200	4.03242300	-0.56288000
C	3.40738700	-1.26213900	1.32002900	C	-2.25106400	2.03749100	-0.96442000
H	5.28074100	-1.98149300	0.54587800	H	-2.37341900	2.96148900	-1.53266300
H	5.22635600	-0.50583300	-1.44671600	H	-2.27485500	1.20070700	-1.65767900
H	3.31328400	1.02508800	-1.80526600	H	-3.08240900	1.95041200	-0.26029200
H	1.54728300	-0.33009600	1.87023400	C	-2.10961500	0.11970100	1.89111000
H	3.43410300	-1.89611600	2.19801400	H	-2.41491000	1.16788800	1.83578400
N	1.23583300	1.36157300	-0.19398700	H	-2.58375200	-0.33561500	2.76193100
H	1.51747700	2.31294600	-0.38568400	H	-1.02962300	0.06643400	2.01461800
C	-0.07632900	1.06120500	-0.32438000	C	-3.86715000	-1.20948500	0.75059200
C	-0.44928100	-0.29282200	-0.58247600	H	-4.25291400	-1.37744900	-0.25131200
C	-1.62220200	-0.94143100	-0.25655900	H	-3.87006800	-2.15434300	1.30095100
N	-0.95879700	2.08385400	-0.26935900	H	-4.51769800	-0.49882500	1.26014200
N	-2.51203300	-0.63625000	0.70046700	Cl	-1.94540200	-2.41281400	-1.16048900

Cartesians coordinates for the optimized structure of (1*Z*,2*E*,3*Z*)-4·H$^+$

(E = -1130.941161; H = -1130.921781; G = -1130.988884)

atom	x	y	z	atom	x	y	z
C	4.54082300	-1.23316000	-0.29906700	H	-2.13714800	1.70479100	0.34482500
C	4.10000900	-1.33999500	1.01859800	C	1.70969500	2.60364500	0.37597700
C	2.82150200	-0.91523800	1.36706700	H	1.61525400	3.66811900	0.59776500
C	1.97601900	-0.39358100	0.38673600	H	1.98156900	2.07768400	1.28716400
C	2.40404600	-0.30006600	-0.93889300	H	2.49924700	2.46212800	-0.36597900
C	3.69126800	-0.71272400	-1.27311700	C	-0.29554400	3.06949900	-0.99487200
H	5.53822100	-1.55970000	-0.56654300	H	0.42527000	3.51268800	-1.68440500
H	4.75332400	-1.74833100	1.78010900	H	-1.05643900	2.55141500	-1.57375700
H	2.48181300	-0.98302300	2.39475900	H	-0.75869900	3.87429000	-0.41533000
H	1.73432500	0.07165300	-1.70522200	C	-4.30339000	0.57428500	0.95157500
H	4.02263600	-0.64293900	-2.30229800	H	-4.56807100	1.42090700	0.30953300
N	0.64489900	-0.02108400	0.76460300	H	-5.21920900	0.14488000	1.35502000
H	0.15532400	-0.70209900	1.32658300	H	-3.68623200	0.92395700	1.77893600
C	-0.13733500	0.96367600	0.25816000	C	-4.45964600	-1.52445700	-0.35591800
C	-1.55856000	0.80209700	0.21269800	H	-3.93455500	-2.10351000	-1.10739400
C	-2.28127400	-0.35677400	-0.01472700	H	-4.79693600	-2.19046700	0.44220600
N	0.41312600	2.12855600	-0.12183500	H	-5.32966600	-1.05570900	-0.81960800
N	-3.59797400	-0.47013300	0.19876300	Cl	-1.48153300	-1.78302100	-0.65484600

Cartesians coordinates for the optimized structure of (1*Z*,2*Z*,3*Z*)-4·H$^+$

(E = -1130.939122; H = -1130.919878; G = -1130.986407)

atom	x	y	z	atom	x	y	z
C	-5.17425900	-0.50877100	0.17584500	H	1.12939800	-1.75380700	0.36102400
C	-4.69189800	-0.73374500	-1.11184200	C	-1.20961100	2.16053000	-0.17040800
C	-3.32128900	-0.76108400	-1.35256300	H	-0.76350200	3.14658100	-0.31274600
C	-2.43093500	-0.57631300	-0.29427400	H	-1.53473500	1.77905900	-1.13435100
C	-2.90656400	-0.36894700	1.00185600	H	-2.07540500	2.25227100	0.48981000
C	-4.27963900	-0.32630900	1.22854300	C	0.60155700	1.90050300	1.47958900
H	-6.24128200	-0.48311500	0.35965000	H	-0.08926800	2.32177200	2.21471600
H	-5.38172600	-0.88225800	-1.93371800	H	1.22619600	1.15671700	1.96688500
H	-2.94376100	-0.92091800	-2.35657600	H	1.22901100	2.70471300	1.08980500
H	-2.21425900	-0.26441300	1.82907700	C	3.53416000	-2.13050700	1.02628200
H	-4.64924500	-0.16855600	2.23471400	H	3.22046000	-3.00766300	0.45036300
N	-1.02450400	-0.67217000	-0.55736800	H	4.51794100	-2.32694800	1.44986200
H	-0.74130600	-1.45940600	-1.12396000	H	2.82907500	-1.96009000	1.83960900
C	0.00051100	0.01728500	0.00570300	C	4.95344900	-0.70642300	-0.41537500
C	1.23583400	-0.69978300	0.14303100	H	4.91976100	0.09022800	-1.14975100
C	2.51730100	-0.24971500	-0.11638500	H	5.66555500	-0.44146500	0.36938900
N	-0.18236400	1.28443900	0.40605200	H	5.28875200	-1.62395700	-0.90478800
N	3.62863700	-0.93684900	0.17757300	Cl	2.74613300	1.29488100	-0.91310800

Cartesians coordinates for the optimized structure of (1*E*,2*E*,3*Z*)-4·H$^+$

(E = -1130.935479; H = -1130.916321; G = -1130.982116)

atom	x	y	z	atom	x	y	z
C	-4.41947500	-1.30398800	0.16219500	H	2.17998100	1.90259800	-0.33481300
C	-3.82737500	-1.56204700	-1.07243500	C	-1.67226500	2.61283500	-0.53307200
C	-2.53912100	-1.11014400	-1.34180300	H	-1.57063100	3.63960600	-0.88996700
C	-1.83256900	-0.40606300	-0.36422400	H	-1.91502100	1.97221100	-1.37601700
C	-2.41504600	-0.15652300	0.88097600	H	-2.48522300	2.56787900	0.19513300
C	-3.71037700	-0.60088700	1.13375100	C	0.26546300	3.26261300	0.85722800
H	-5.42469000	-1.65083000	0.36698500	H	-0.48727400	3.75102100	1.47842800
H	-4.37049800	-2.10919200	-1.83342600	H	1.02668300	2.83178800	1.50335500
H	-2.08604400	-1.29592900	-2.30974700	H	0.72200700	4.01698100	0.20878800
H	-1.86320500	0.37044300	1.65014300	C	2.99485500	-2.54404900	0.25643600
H	-4.16005300	-0.40600500	2.10004900	H	3.79440000	-2.60321600	0.99984200
N	-0.48814900	-0.01380300	-0.65613400	H	2.35363200	-3.42012400	0.35148500
H	0.04543200	-0.67593600	-1.20091100	H	3.43004300	-2.53621900	-0.73912100
C	0.22574400	1.05605200	-0.21125400	C	1.11833700	-1.50294000	1.49494800
C	1.65066500	0.97910800	-0.15368800	H	0.85641000	-0.53124000	1.90870000
C	2.44672400	-0.15098200	-0.05634400	H	0.22319500	-1.97732000	1.08800400
N	-0.39263300	2.21500800	0.06846500	H	1.51612700	-2.13005100	2.29484300
N	2.16489700	-1.34719500	0.47590700	Cl	4.08897500	0.05103300	-0.64680600

Cartesians coordinates for the optimized structure of (1*E*,2*Z*,3*Z*)-4·H$^+$

(E = -1130.933296; H = -1130.914249; G = -1130.979670)

atom	x	y	z	atom	x	y	z
C	5.16157900	-0.29408400	-0.25807100	H	-0.97747500	-2.03910100	0.12605100
C	4.75666800	-0.23689200	1.07396000	C	1.00990100	2.08556100	-0.27446800
C	3.40512300	-0.30829900	1.39945700	H	0.51044700	3.05293100	-0.35135700
C	2.45871500	-0.45172100	0.38466000	H	1.39749000	1.96715800	0.73406500
C	2.85766200	-0.52931700	-0.95071900	H	1.84354700	2.06113300	-0.98029200
C	4.21091100	-0.43952400	-1.26646200	C	-0.84938900	1.32029200	-1.71365800
H	6.21352100	-0.23464800	-0.50885000	H	-0.24483600	1.76300700	-2.50784000
H	5.49160800	-0.13175100	1.86273600	H	-1.29423500	0.39978700	-2.08330500
H	3.08573300	-0.25182000	2.43424200	H	-1.64211100	2.02606700	-1.45012800
H	2.12403400	-0.68302400	-1.73359300	C	-2.38657200	1.45606600	1.40284600
H	4.52254700	-0.50395300	-2.30209400	H	-1.92460500	2.30262400	0.88945000
N	1.07574400	-0.58867200	0.74834400	H	-3.12767700	1.83825000	2.10640700
H	0.88172600	-1.29234700	1.44771600	H	-1.62640600	0.91031300	1.95878600
C	-0.02231100	-0.13297200	0.09281900	C	-4.45789700	0.91502100	0.14677800
C	-1.17844900	-0.97673500	0.12314700	H	-4.74941500	0.51231400	-0.81942700
C	-2.51347800	-0.61417800	0.11214600	H	-5.14191600	0.54324500	0.91440100
N	0.02308400	1.03836700	-0.56994600	H	-4.52347500	2.00196000	0.10697900
N	-3.06657200	0.55257200	0.46680500	Cl	-3.63288600	-1.88337300	-0.35264600

Cartesians coordinates for the optimized structure of *trans*-5

(E = -1130.502907; H = -1130.484726; G = -1130.547267)

atom	x	y	z	atom	x	y	z
C	2.93721300	1.80187700	-0.59286200	C	-3.90718400	1.31974000	0.32156100
C	2.39803500	0.59409500	-0.82748600	H	-4.28384200	1.09366200	1.33074400
C	0.92494300	0.34954500	-0.71851700	H	-3.28234000	2.20577900	0.37008100
C	0.11506300	1.52053800	-0.17872000	H	-4.76545300	1.51822000	-0.32647200
C	0.78311900	2.78487900	0.03546500	C	-3.85753600	-1.03339700	-0.38437300
C	2.11572700	2.91566500	-0.15829300	H	-4.86406600	-0.81213300	-0.74445300
H	4.00089500	1.96217800	-0.72838400	H	-3.35783900	-1.66605300	-1.12041300
H	3.00772000	-0.22948000	-1.17841400	H	-3.94774400	-1.60182900	0.55504500
H	0.55737000	0.23693300	-1.75211300	C	0.53077000	-0.65388500	2.38118000
H	0.16722500	3.61004400	0.37260200	H	0.76362700	-1.23159100	3.27953300
H	2.59384800	3.87321300	0.01831600	H	1.01244400	0.33326700	2.48184300
N	-1.15636700	1.42703200	0.03497900	H	-0.54644500	-0.51407700	2.33468700
C	-1.75726600	0.16998800	-0.09244000	C	2.43177100	-1.68061100	1.32082800
C	-1.03991200	-0.99041400	-0.03330000	H	2.76183200	-2.29249900	0.48472300
C	0.44850700	-0.98766800	-0.05254700	H	3.04940400	-0.77013600	1.36394100
N	-3.13330700	0.21125500	-0.22442200	H	2.60259200	-2.24661800	2.24084100
N	1.00374300	-1.40017400	1.21481800	Cl	0.95896800	-2.34412200	-1.31862500
H	-1.50966000	-1.94770400	0.13391500				

Cartesians coordinates for the optimized structure of *cis*-5

(E = -1130.522610; H = -1130.503839; G = -1130.567986)

atom	x	y	z	atom	x	y	z
C	-2.99856900	-1.53826600	-0.86807300	C	3.81088300	-1.56556700	0.19846700
C	-2.39007700	-0.35259100	-1.04250800	H	4.34197400	-1.44696300	1.14909900
C	-0.90824900	-0.21048600	-0.89813100	H	3.08048000	-2.36207200	0.29088300
C	-0.20621500	-1.40742300	-0.30142400	H	4.53717600	-1.81914700	-0.57990900
C	-0.94264000	-2.62864800	-0.13185400	C	3.95384400	0.86543800	-0.22999500
C	-2.26586500	-2.69367400	-0.41173900	H	4.96341500	0.56558600	-0.51303200
H	-4.06137200	-1.63439600	-1.05711400	H	3.57443500	1.54767500	-0.99247600
H	-2.94582300	0.49382200	-1.42154800	H	4.00948100	1.39929300	0.72720000
H	-0.55516300	-0.21338900	-1.95631300	C	-0.19891700	3.50356400	-0.33898300
H	-0.39120600	-3.47944500	0.24659900	H	-0.88210300	4.30872300	-0.61226600
H	-2.80162400	-3.62474100	-0.26569800	H	0.21046900	3.71925200	0.65606000
N	1.09440600	-1.42187800	-0.13253500	H	0.61320300	3.48089400	-1.06644600
C	1.76814900	-0.24759600	-0.20948800	C	-2.30051300	2.35687300	0.19013900
C	1.11391200	1.00918400	-0.24865000	H	-2.59076000	1.42225800	0.66225800
C	-0.26424100	1.07412100	-0.39315300	H	-2.28064900	3.10856000	0.98267700
N	3.12195600	-0.32450000	-0.14735600	H	-3.01660000	2.67349200	-0.57535900
N	-0.94055100	2.24571800	-0.36425100	Cl	-1.14249600	-0.14766100	2.16965200
H	1.65741900	1.88586300	0.06265200				

Cartesians coordinates for the optimized structure of *trans*-5·H$^+$

(E = -1130.876947; H = -1130.858590; G = -1130.921342)

atom	x	y	z	atom	x	y	z
C	2.99021700	1.76727800	-0.58553700	H	-1.51997900	-1.97767100	0.07498400
C	2.41500000	0.56968800	-0.84866000	C	-3.89870900	1.34424000	0.27283600
C	0.95513000	0.35656100	-0.71123700	H	-4.94739300	1.21014600	0.01623900
C	0.19574600	1.52233700	-0.19269000	H	-3.83121100	1.46715200	1.36196000
C	0.83633300	2.75183600	0.06013500	H	-3.58510000	2.26758500	-0.22293600
C	2.19107900	2.86270100	-0.13575300	C	-3.88370200	-1.07947900	-0.29747100
H	4.05386200	1.91200500	-0.72560500	H	-4.90886700	-0.87345400	-0.59995200
H	2.99560000	-0.25747800	-1.23687100	H	-3.42995900	-1.72245000	-1.05302100
H	0.56247800	0.20786900	-1.73233000	H	-3.89993800	-1.61466100	0.66080300
H	0.25684600	3.60054000	0.40596500	C	0.58596200	-0.52947200	2.32518300
H	2.67164900	3.81507700	0.05786400	H	-0.48914000	-0.36606800	2.32088200
N	-1.12220700	1.37031400	-0.03697400	H	0.84805400	-1.01435300	3.26570100
H	-1.66519300	2.17914300	0.23299700	H	1.10465700	0.44476600	2.29563700
C	-1.78756800	0.11701900	-0.10735100	C	2.38226900	-1.81297100	1.33174300
C	-1.04515000	-1.01757300	-0.04591400	H	2.61851000	-2.58372900	0.60403700
C	0.45309100	-1.03902600	-0.05269900	H	3.07639000	-0.96647300	1.19881900
N	-3.15431100	0.18517300	-0.22337500	H	2.54103500	-2.22490700	2.32860800
N	0.98488800	-1.40014200	1.22041200	Cl	0.95593600	-2.32172300	-1.29704300

Cartesians coordinates for the optimized structure of *cis*-5·H$^+$

(E = -1130.879260; H = -1130.860378; G = -1130.924679)

atom	x	y	z	atom	x	y	z
C	-2.90646500	1.92690000	0.51836300	H	1.39793200	-1.98126200	-0.25939700
C	-2.41024900	0.69376600	0.75288200	C	3.95247800	1.25892100	0.08620100
C	-0.95730800	0.39712900	0.68205500	H	4.98763900	1.00977600	0.30754500
C	-0.11515900	1.55447600	0.28217700	H	3.92781300	1.71099300	-0.91442300
C	-0.67147600	2.83063900	0.06410400	H	3.64343700	1.99542000	0.83331300
C	-2.02647500	3.00190300	0.17117400	C	3.82445600	-1.24983300	0.01662800
H	-3.96863400	2.12015300	0.59683800	H	4.88433900	-1.12223800	0.22412800
H	-3.06730900	-0.11100600	1.04968400	H	3.42582500	-1.97539300	0.72952900
H	-0.63085300	0.12164600	1.70480700	H	3.71015600	-1.64890300	-0.99771400
H	-0.02879600	3.65883200	-0.21250500	C	-0.73542200	-2.83694400	1.39850000
H	-2.44833500	3.98292800	-0.01603800	H	-1.14210600	-2.38321700	2.31672900
N	1.19590900	1.34271100	0.13980800	H	-1.10532500	-3.86161800	1.34025000
H	1.77070700	2.13233900	-0.12424700	H	0.34866800	-2.86199300	1.48745100
C	1.79081800	0.06174700	0.11802400	C	-2.54822000	-2.37642200	-0.16428200
C	0.97263700	-1.02413900	-0.00369800	H	-2.84669100	-1.76513700	-1.01061500
C	-0.49866000	-0.91424300	-0.12095200	H	-2.64556000	-3.42501400	-0.45656000
N	3.15292100	0.03835600	0.17976700	H	-3.23422300	-2.20415700	0.67617400
N	-1.15227100	-2.12395100	0.19159800	Cl	-0.90472500	-0.47855100	-1.98001200

Cartesians coordinates for the optimized structure of TS$^{‡}_{trans\text{-}5}$

(E = -1130.480688; H = -1130.462213; G = -1130.525523)

atom	x	y	z
C	2.84738900	1.97676400	-0.50878400
C	2.26053100	0.87414100	-1.06545600
C	0.84932600	0.65060700	-0.93871200
C	0.04220600	1.63062700	-0.25450900
C	0.68525100	2.79910300	0.26052100
C	2.04122600	2.95407200	0.14556600
H	3.91596300	2.13724200	-0.59586800
H	2.84917400	0.16130100	-1.63311500
H	0.35614600	0.17025000	-1.77253700
H	0.06834700	3.53962100	0.75611500
H	2.51627100	3.83826600	0.55788100
N	-1.25898900	1.44254100	-0.06021500
C	-1.76567400	0.19092100	-0.01804700
C	-1.00023300	-0.95955500	0.28089500
C	0.39325400	-1.15870000	0.04599300
N	-3.13662400	0.09132200	-0.05368600
N	1.19549800	-1.49078600	1.11701100
H	-1.42782200	-1.65297800	0.99790900

atom	x	y	z
C	-3.99449700	1.25663600	0.09888700
H	-4.52343300	1.23161300	1.06157200
H	-3.38498300	2.15362200	0.04967800
H	-4.74207600	1.27960800	-0.70103500
C	-3.80070400	-1.19512000	0.01272400
H	-4.75470500	-1.13000600	-0.51764900
H	-3.18359300	-1.95640500	-0.46551900
H	-4.01089200	-1.51418600	1.04446800
C	1.14690600	-0.57838000	2.26423900
H	1.21790000	-1.15424000	3.19075400
H	1.97771600	0.13724500	2.22713200
H	0.20768800	-0.03283000	2.26332700
C	2.46743100	-2.19845500	1.00309800
H	2.35963700	-3.10508400	0.41458800
H	3.24224500	-1.56739300	0.54825600
H	2.79166000	-2.47258500	2.00840500
Cl	0.81712300	-2.22473900	-1.43615400

Cartesians coordinates for the optimized structure of TS$^{‡}_{cis\text{-}5}$

(E = -1130.481235; H = -1130.461861; G = -1130.528435)

atom	x	y	z
C	-2.87398600	-1.93644700	-0.66514800
C	-2.25049400	-0.87406200	-1.26974000
C	-0.85774300	-0.66139200	-1.09418900
C	-0.08610800	-1.60062700	-0.34641400
C	-0.75290800	-2.71701700	0.22583500
C	-2.10946500	-2.86456700	0.08464900
H	-3.94021300	-2.08970900	-0.78349700
H	-2.81525900	-0.20101200	-1.90549200
H	-0.33279300	-0.05460500	-1.82342400
H	-0.16093700	-3.42070400	0.79751700
H	-2.60871000	-3.70560000	0.55321100
N	1.23665100	-1.44727100	-0.15232300
C	1.78528000	-0.24717600	-0.07556600
C	1.04738900	0.96002000	0.19937500
C	-0.32605200	1.10808200	0.14425400
N	3.15497100	-0.16834700	-0.13199700
N	-1.01951100	2.12439600	-0.32879500
H	1.51511300	1.63683000	0.91001200

atom	x	y	z
C	3.97064700	-1.37565500	-0.12404300
H	4.75720400	-1.29470000	-0.88049200
H	4.44386600	-1.52527400	0.85519000
H	3.33994700	-2.23184000	-0.34207600
C	3.86692500	1.07587900	0.09230800
H	4.84672400	1.00863900	-0.38547900
H	3.32772200	1.91125900	-0.35632800
H	4.02394900	1.29212900	1.15839900
C	-0.41331000	3.12155100	-1.21815400
H	-0.71115300	2.93867700	-2.25703500
H	-0.76319800	4.11561800	-0.92750400
H	0.66826500	3.06611800	-1.14028200
C	-2.46819600	2.26922500	-0.16796800
H	-2.86888000	1.39855600	0.33803100
H	-2.67762900	3.15541300	0.43653000
H	-2.92661400	2.39285200	-1.15414100
Cl	-1.28906200	0.61758900	2.14632200

Cartesians coordinates for the optimized structure of $TS^{\ddagger}_{trans\text{-}5\cdot H}$

(E = -1130.876393; H = -1130.858126; G = -1130.920627)

atom	x	y	z	atom	x	y	z
C	3.01873300	1.75673400	-0.54252900	H	-1.62979800	-1.92678200	-0.09564300
C	2.34063200	0.69382300	-1.06925900	C	-3.84906600	1.30073200	-0.66825900
C	0.91937500	0.52270300	-0.85271700	H	-4.11235100	0.88555100	-1.64916000
C	0.23759100	1.55465500	-0.09671700	H	-4.76370700	1.60303400	-0.15731500
C	0.95401700	2.64769500	0.42210800	H	-3.23448000	2.18441700	-0.83038500
C	2.31195100	2.74072300	0.19365300	C	-3.91982700	-0.90661200	0.39782600
H	4.08197400	1.87388500	-0.70866900	H	-4.93060200	-0.61548900	0.68305700
H	2.84668400	-0.03217900	-1.69433100	H	-3.98370400	-1.54962700	-0.49081200
H	0.37699800	0.23883600	-1.75259400	H	-3.48222000	-1.47517000	1.21873300
H	0.43688700	3.41594100	0.98614900	C	0.60675200	-0.74555200	2.31087000
H	2.85310800	3.59193400	0.59106500	H	-0.47047300	-0.60560300	2.32168000
N	-1.09378900	1.41678000	0.11073800	H	0.88715100	-1.34532000	3.17614900
H	-1.55650400	2.11352600	0.68084500	H	1.10474500	0.23084400	2.38711500
C	-1.77727500	0.17545300	0.01888300	C	2.40818500	-1.91732400	1.11369400
C	-1.09413800	-0.98999800	-0.05768500	H	2.53888600	-2.77292700	0.45703800
C	0.39253200	-1.13237800	-0.08226900	H	3.09217600	-1.11676800	0.80006100
N	-3.14266900	0.30600700	0.15623800	H	2.66012000	-2.21383500	2.13010000
N	1.01965500	-1.45236500	1.09593800	Cl	0.85329200	-2.26947900	-1.41876900

Cartesians coordinates for the optimized structure of $TS^{\ddagger}_{cis\text{-}5\cdot H}$

(E = -1130.877825; H = -1130.859428; G = -1130.922243)

atom	x	y	z	atom	x	y	z
C	2.95613500	1.83837400	-0.52948600	H	-1.51782100	-1.94301800	0.17941700
C	2.34271200	0.71989600	-1.00700500	C	-3.92597300	1.12038100	-0.75125900
C	0.91801500	0.49691800	-0.83334000	H	-4.23771400	0.62398500	-1.67856500
C	0.15967100	1.58131400	-0.23410900	H	-4.81606000	1.45369400	-0.21612400
C	0.80826400	2.74345300	0.21498900	H	-3.33413600	1.99288900	-1.02093000
C	2.17464200	2.85465500	0.08257000	C	-3.88199000	-1.01244200	0.47006700
H	4.02247000	1.98218400	-0.64670700	H	-4.90196700	-0.73739200	0.73785700
H	2.91048200	-0.01763500	-1.56063500	H	-3.92593800	-1.73794800	-0.35369500
H	0.43705200	0.07899100	-1.71886700	H	-3.41509200	-1.47941800	1.33726700
H	0.23425600	3.53669200	0.68033300	C	0.65418100	-2.69949400	-1.55082400
H	2.66653400	3.74840500	0.44931300	H	1.13899300	-2.20062800	-2.40230200
N	-1.17074500	1.41119200	-0.04570600	H	0.92811600	-3.75401400	-1.57004400
H	-1.65938600	2.13629700	0.46474000	H	-0.42272000	-2.61074800	-1.67115300
C	-1.79361100	0.13897300	-0.00449000	C	2.44722800	-2.43761600	0.14743500
C	-1.03696700	-0.98618200	0.04584900	H	2.45896700	-2.79283100	1.17735300
C	0.44224600	-0.99015600	0.17995000	H	2.83619200	-3.21940300	-0.50154700
N	-3.15914400	0.20169000	0.10310200	H	3.10493000	-1.56446500	0.08149900
N	1.07860300	-2.12110100	-0.27430200	Cl	0.98026700	-0.59685600	1.90406200

Cartesians coordinates for the optimized structure of (1*Z*-3*E*)-4

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.547191; H = -1130.527813; G = -1130.595172)

atom	x	y	z
C	4.00510200	0.69867300	-0.27468400
C	3.69532900	0.05744400	0.92574800
C	2.53955500	-0.70812900	1.04032300
C	1.64770200	-0.84159100	-0.03918400
C	1.97790800	-0.20129100	-1.24876800
C	3.14110800	0.55645700	-1.36048700
H	4.90984500	1.28875200	-0.36587400
H	4.36097100	0.14955800	1.77758800
H	2.30360900	-1.21748600	1.96778200
H	1.32668600	-0.32226600	-2.10658400
H	3.37637400	1.03382300	-2.30622600
N	0.55098300	-1.69303100	0.10318300
C	-0.65558900	-1.38317400	-0.25333800
C	-1.13478000	-0.02785200	-0.63278900
C	-1.11645200	1.08183000	0.12761100
N	-1.58429000	-2.39192800	-0.35873800
N	-1.32742200	2.37054000	-0.29302000
H	-1.54409600	0.06782100	-1.63218200
C	-1.16065600	-3.76576500	-0.12415600
H	-1.88640700	-4.43925800	-0.58444800
H	-0.17857100	-3.92847200	-0.56277300
H	-1.09666700	-3.99755200	0.94703200
C	-3.01777900	-2.15994100	-0.22334600
H	-3.36936900	-2.43666900	0.77939400
H	-3.25074500	-1.11130200	-0.38865900
H	-3.56315600	-2.76232400	-0.95493000
C	-1.34530900	2.60641900	-1.73396800
H	-2.27676800	2.26384700	-2.20714100
H	-1.24771600	3.67878200	-1.90787200
H	-0.50322100	2.09597700	-2.20071700
C	-2.19807900	3.26971900	0.46921500
H	-3.25750100	3.10022000	0.23339800
H	-2.04945500	3.12774500	1.53635200
H	-1.94487300	4.30062800	0.21813800
Cl	-0.69718900	0.94190100	1.85674600

Cartesians coordinates for the optimized structure of (1*E*-3*E*)-4

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.546726; H = -1130.527411; G = -1130.593532)

atom	x	y	z
C	3.65981500	-1.29077900	-0.49033100
C	3.13245000	-1.66972900	0.74458000
C	1.75514900	-1.73396100	0.93520800
C	0.86044400	-1.40053700	-0.09874100
C	1.40659200	-1.03903700	-1.34662000
C	2.78468500	-0.98549900	-1.53368200
H	4.73228500	-1.24931400	-0.64211700
H	3.79689500	-1.92721300	1.56277500
H	1.34676100	-2.05247900	1.88779300
H	0.74064200	-0.81484900	-2.17116300
H	3.17797500	-0.70833100	-2.50632600
N	-0.50665800	-1.56418300	0.12650800
C	-1.41843400	-0.71789600	-0.24951700
C	-1.18502200	0.67179400	-0.71225300
C	-0.36787100	1.56943700	-0.12629400
N	-2.72396500	-1.14803700	-0.28882900
N	0.13340900	1.60351900	1.13013300
H	-1.69262200	0.97004700	-1.61978500
C	-3.01878500	-2.54519300	-0.00017400
H	-3.98780900	-2.79546300	-0.43680900
H	-2.24732300	-3.18081100	-0.42868200
H	-3.06024400	-2.74011200	1.07948900
C	-3.85958000	-0.24313300	-0.15211500
H	-4.27421700	-0.28444100	0.86391400
H	-3.56226300	0.78218500	-0.35621100
H	-4.64874100	-0.52627300	-0.85379500
C	-0.58276900	0.95633700	2.22537100
H	-0.28448000	-0.08788300	2.36122300
H	-0.37334500	1.50798700	3.14469200
H	-1.65454400	0.99122900	2.03031800
C	1.49361000	2.04572000	1.43702500
H	2.12514100	1.18796200	1.68858700
H	1.92724100	2.55591000	0.58157600
H	1.47360600	2.73388300	2.28631800
Cl	0.01081300	3.04080800	-1.12007200

Cartesians coordinates for the optimized structure of (1*E*-2*E*-3*E*)-4•H

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.994685; H = -1130.975435; G = -1131.041251)

atom	x	y	z
C	3.49104600	-1.61373000	-0.65815500
C	3.05674700	-1.94786900	0.62251400
C	1.70919700	-1.83994100	0.95764000
C	0.78579400	-1.40565500	0.00339300
C	1.21252300	-1.09423900	-1.29056600
C	2.56381100	-1.18893800	-1.60959800
H	4.54002700	-1.69270700	-0.91687600
H	3.76484500	-2.29033300	1.36772300
H	1.37380000	-2.10059600	1.95515500
H	0.49717200	-0.79025600	-2.04325400
H	2.88881100	-0.94561200	-2.61431100
N	-0.59318300	-1.36907500	0.36894200
H	-0.89721700	-2.12914000	0.96206300
C	-1.55830400	-0.51854100	-0.07269000
C	-1.26753500	0.80581800	-0.52982900
C	-0.24589600	1.62485800	-0.10209000
N	-2.81511200	-0.98133500	-0.11960400
N	0.40287600	1.62287600	1.06387500
H	-1.87556300	1.17443200	-1.34232600
C	-3.13478400	-2.41251500	-0.07727800
H	-4.00820300	-2.58616000	-0.70574800
H	-2.30580500	-2.99819000	-0.47038600
H	-3.36956800	-2.73967400	0.94002000
C	-3.97198500	-0.08451400	-0.21056100
H	-4.74496400	-0.44428800	0.47033100
H	-3.69097400	0.92466700	0.07830500
H	-4.37373100	-0.07676800	-1.22721900
C	-0.22084200	1.08492100	2.27815700
H	0.18594100	0.10569000	2.53649100
H	-0.01768600	1.77823200	3.09588500
H	-1.29705000	1.00876900	2.13831800
C	1.70216900	2.27733100	1.27300800
H	2.27257600	2.30472500	0.34954000
H	1.56391700	3.29399300	1.65057700
H	2.25691900	1.69586300	2.00859600
Cl	0.20841400	2.91048100	-1.23112000

Cartesians coordinates for the optimized structure of (1*Z*-2*Z*-3*E*)-4•H

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.997848; H = -1130.979370; G = -1131.043902)

atom	x	y	z
C	-4.21958200	-1.52622300	-0.42293800
C	-4.36789400	-0.58455900	0.59343400
C	-3.37538000	0.36595100	0.81935200
C	-2.23339600	0.38012700	0.01582100
C	-2.08895000	-0.54782900	-1.01877600
C	-3.07887100	-1.50397400	-1.22522600
H	-4.99043200	-2.26800400	-0.59430300
H	-5.25292900	-0.59076100	1.21849900
H	-3.48072900	1.09134600	1.61808500
H	-1.21699500	-0.51432100	-1.65933800
H	-2.96429400	-2.22320100	-2.02764200
N	-1.25627000	1.39632300	0.23849500
H	-1.62514500	2.31614000	0.43737000
C	0.08641400	1.23008800	0.32357300
C	0.59142200	-0.08285700	0.59051100
C	1.69270500	-0.70501600	0.04702400
N	0.85072700	2.32573800	0.20550700
N	2.20769500	-1.85748100	0.49765700
H	-0.05158700	-0.69407700	1.20878500
C	0.32466200	3.57764500	-0.34922000
H	1.14734800	4.11050200	-0.82515600
H	-0.43399200	3.36822900	-1.10143300
H	-0.09499100	4.21872200	0.43305700
C	2.19060600	2.43516700	0.78926600
H	2.21321100	3.31210300	1.44029200
H	2.41970200	1.55254700	1.37900300
H	2.94024900	2.55661600	0.00539400
C	1.73927200	-2.39281400	1.78031400
H	0.79178300	-2.92954300	1.66721200
H	2.49117100	-3.08599000	2.15408100
H	1.61346900	-1.58344900	2.49868400
C	3.04185000	-2.77680900	-0.28380400
H	3.30193200	-2.34574700	-1.24362500
H	3.95659400	-2.99436700	0.27082900
H	2.49607200	-3.70969300	-0.44852700
Cl	2.48866800	0.00867700	-1.35169900

Cartesians coordinates for the optimized structure of (1*Z*-2*E*-3*E*)-4•H

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.996972; H = -1130.977537; G = -1131.044418)

atom	x	y	z
C	-3.97594600	0.06274000	0.65016400
C	-3.76499000	-0.52364300	-0.59611800
C	-2.51687400	-1.04504100	-0.92541500
C	-1.47396800	-0.99268800	0.00271200
C	-1.68650200	-0.42800500	1.26291000
C	-2.93304700	0.10695600	1.57477200
H	-4.94597100	0.47383500	0.90265100
H	-4.56958800	-0.57031700	-1.32039300
H	-2.34828900	-1.48682400	-1.90113100
H	-0.89062700	-0.41681500	1.99599200
H	-3.09266300	0.54341100	2.55380900
N	-0.23141100	-1.59361500	-0.34881900
H	-0.30872900	-2.42872800	-0.91268900
C	1.02099600	-1.22904600	0.02764100
C	1.37708600	0.11315200	0.36900800
C	0.94694800	1.28248600	-0.22346800
N	1.94360400	-2.19941000	0.10838600
N	1.12041800	2.49894700	0.30666900
H	2.11353800	0.21585600	1.15278200
C	1.59209200	-3.62245100	0.15849700
H	2.31548400	-4.13192600	0.79486100
H	0.60065400	-3.75326200	0.58854100
H	1.62536600	-4.07688000	-0.83623500
C	3.38081500	-1.90827500	0.12849200
H	3.89298200	-2.64901400	-0.48704200
H	3.57052100	-0.91980100	-0.28163300
H	3.77384400	-1.96480100	1.14739300
C	1.57086500	2.61983000	1.69767600
H	2.65777000	2.51535500	1.77502400
H	1.28772100	3.60656800	2.06075900
H	1.08831400	1.86361600	2.31492000
C	1.08678200	3.76295400	-0.43759800
H	0.88217700	3.59124100	-1.48801700
H	0.31295400	4.41093700	-0.02091600
H	2.05544400	4.25917400	-0.34046600
Cl	0.14148700	1.22253500	-1.78220600

Cartesians coordinates for the optimized structure of (1*E*-2*Z*-3*E*)-4•H

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.994103; H = -1130.974983; G = -1131.040832)

atom	x	y	z
C	4.49557700	-1.33634800	0.37765300
C	4.57145300	-0.30668400	-0.55847100
C	3.48718900	0.54362800	-0.75577400
C	2.32240100	0.37066400	-0.00336600
C	2.24757000	-0.64859800	0.94888700
C	3.33156900	-1.50371600	1.12633600
H	5.33862000	-2.00016100	0.52672200
H	5.47224700	-0.16646500	-1.14395700
H	3.53917100	1.33565900	-1.49445000
H	1.35847700	-0.76891400	1.55302300
H	3.26862400	-2.29394200	1.86498300
N	1.25606400	1.29939500	-0.19618400
H	1.55005100	2.24874000	-0.38026600
C	-0.06499400	1.03252300	-0.32791500
C	-0.48027300	-0.30726400	-0.60946000
C	-1.66624000	-0.91242300	-0.26295500
N	-0.91600600	2.07270800	-0.25295700
N	-2.52954800	-0.58852500	0.70691700
H	0.23062200	-0.90669300	-1.15928300
C	-0.49549200	3.37608500	0.27533200
H	-1.37311500	3.87850800	0.67983500
H	0.22648500	3.24473900	1.08015100
H	-0.06731100	4.00990100	-0.50857200
C	-2.21781500	2.07220100	-0.93113900
H	-2.30857800	3.00105600	-1.49649900
H	-2.28217400	1.23671200	-1.62234700
H	-3.03987700	2.01926900	-0.21407600
C	-2.08944100	0.13738400	1.90419600
H	-2.36549800	1.19348700	1.86521500
H	-2.57026300	-0.31823900	2.77079800
H	-1.01129200	0.05132000	2.01633400
C	-3.91917200	-1.06699600	0.74511700
H	-4.29983800	-1.22584600	-0.25969300
H	-3.99187100	-1.99651300	1.31593400
H	-4.52587700	-0.30323200	1.23082500
Cl	-2.05624500	-2.37806900	-1.17645500

Cartesians coordinates for the optimized structure of *trans*-5

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.572776; H = -1130.553791; G = -1130.619657)

atom	x	y	z
C	2.61606100	1.55899000	1.54372800
C	2.11130000	0.34454500	1.25760400
C	0.91561400	0.20557600	0.36659400
C	0.05849400	1.43445700	0.31438800
C	0.72477700	2.69811500	0.50019000
C	1.94650500	2.75322700	1.08876000
H	3.52041600	1.65194900	2.13236300
H	2.60734300	-0.54809000	1.60859200
H	1.37952700	0.23997500	-0.69360100
H	0.16889000	3.59360600	0.25263900
H	2.40866300	3.71561200	1.27745400
N	-1.22438600	1.43920400	0.07482900
C	-1.89111900	0.24138200	0.06100900
C	-1.24613000	-0.99979100	0.28411900
C	0.13202500	-1.07538200	0.40892600
N	-3.21303800	0.30049800	-0.17609100
N	0.76862000	-2.25839700	0.55044300
H	-1.82869000	-1.90412900	0.26210100
C	-3.90763700	1.55466300	-0.47751300
H	-4.68597700	1.73217100	0.26918500
H	-3.19799800	2.37351500	-0.46645100
H	-4.37478600	1.48508100	-1.46334800
C	-4.03634400	-0.90865400	-0.17534200
H	-5.07011500	-0.62144000	-0.35156600
H	-3.72859900	-1.59747800	-0.96698700
H	-3.98048100	-1.42255500	0.78732100
C	0.00076800	-3.48122300	0.78303900
H	-0.46301600	-3.85253300	-0.13822400
H	0.68089200	-4.24376600	1.16061800
H	-0.77198300	-3.31019900	1.53233300
C	2.14992400	-2.50004300	0.11014900
H	2.56254000	-1.63617400	-0.40199800
H	2.78694800	-2.78336100	0.95242300
H	2.14002900	-3.32424000	-0.60730800
Cl	2.24015300	0.18398500	-2.62845500

Cartesians coordinates for the optimized structure of *cis*-5

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.559316; H = -1130.540292; G = -1130.606166)

atom	x	y	z
C	-2.86753000	-1.65975000	-1.07094100
C	-2.26750900	-0.47395200	-1.27365700
C	-0.80333500	-0.29067600	-1.02786000
C	-0.09107900	-1.47133400	-0.40863400
C	-0.81483800	-2.69732100	-0.23152600
C	-2.13517400	-2.78054900	-0.53226000
H	-3.91258600	-1.79073100	-1.32318000
H	-2.80719600	0.33799600	-1.73932400
H	-0.39725900	-0.28714500	-2.06295000
H	-0.26887900	-3.53628200	0.18070200
H	-2.66341600	-3.71274400	-0.36844000
N	1.17414700	-1.43073300	-0.09433200
C	1.83338300	-0.23173000	-0.16035500
C	1.14321800	1.00423500	-0.26932000
C	-0.21452000	1.03401300	-0.53604000
N	3.16821000	-0.27294100	-0.01460900
N	-0.92052300	2.17764600	-0.56085300
H	1.64740500	1.90814400	0.02970600
C	3.88769900	-1.49779700	0.34212900
H	4.41766400	-1.34465200	1.28609400
H	3.18440200	-2.31579100	0.44601100
H	4.61748200	-1.73414200	-0.43634800
C	3.98111600	0.93904000	-0.08920400
H	5.00826600	0.65102000	-0.30742400
H	3.62778800	1.59026900	-0.88885600
H	3.96725200	1.48991700	0.85692000
C	-0.22582600	3.46718900	-0.58106900
H	-0.92060400	4.22058000	-0.95190900
H	0.10820400	3.76350600	0.41928500
H	0.63110700	3.42419700	-1.25252800
C	-2.33066300	2.27046100	-0.15152800
H	-2.66147700	1.34287800	0.30312800
H	-2.40296200	3.04202100	0.61742300
H	-2.96989900	2.55405700	-0.99198600
Cl	-1.57222200	0.08283100	2.75375400

Cartesians coordinates for the optimized structure of *trans*-5•H

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.937068; H = -1130.918974; G = -1130.980660)

atom	x	y	z	atom	x	y	z
C	2.99036900	1.78129100	-0.55021900	H	-1.51379600	-1.97869300	0.02584500
C	2.42972500	0.57773000	-0.80360100	C	-3.89311500	1.36491000	0.21393200
C	0.96553100	0.35702800	-0.68655900	H	-4.93665500	1.22631100	-0.05928700
C	0.19338100	1.52270200	-0.17130400	H	-3.84126600	1.51990900	1.29846300
C	0.82510600	2.75860300	0.07582600	H	-3.55873500	2.26760000	-0.30254500
C	2.17854600	2.87413500	-0.11072000	C	-3.87604800	-1.07962600	-0.27349000
H	4.05363800	1.93381400	-0.68089100	H	-4.90907300	-0.87664100	-0.54841700
H	3.02185400	-0.24828600	-1.17437300	H	-3.44194600	-1.73204900	-1.03290100
H	0.60002200	0.25551300	-1.72480000	H	-3.86384100	-1.60431800	0.69029800
H	0.23693000	3.60385600	0.41178800	C	0.47764000	-0.68341700	2.36085100
H	2.65206800	3.82962500	0.08197500	H	-0.60696500	-0.61581600	2.34278700
N	-1.12001600	1.36798000	-0.02087800	H	0.77025500	-1.21490100	3.26703700
H	-1.66297700	2.17584300	0.25472800	H	0.90490900	0.33136500	2.41470600
C	-1.78268300	0.11902000	-0.12078000	C	2.40528600	-1.71240200	1.32790200
C	-1.03839700	-1.01778000	-0.08283100	H	2.74509600	-2.35668300	0.52138200
C	0.45351700	-1.02122300	-0.06047000	H	3.00939900	-0.79189600	1.33021500
N	-3.14658600	0.18440200	-0.22901700	H	2.57564500	-2.22953300	2.27325500
N	0.97446900	-1.43727600	1.20443800	Cl	0.99042500	-2.31450500	-1.34013500

Cartesians coordinates for the optimized structure of *cis*-5•H

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.975810; H = -1130.956841; G = -1131.021387)

atom	x	y	z	atom	x	y	z
C	3.09165400	1.40300200	-0.89908000	H	-1.70095600	-1.92570100	-0.07231700
C	2.45270300	0.22052600	-1.02156000	C	-3.72794400	1.62161200	0.12366700
C	0.97246400	0.12363000	-0.87755900	H	-4.80543200	1.49123000	0.12239300
C	0.32136900	1.35792300	-0.35288600	H	-3.43107900	1.97834800	1.11377000
C	1.03530000	2.56931400	-0.25874300	H	-3.48411800	2.36756900	-0.63642500
C	2.37548400	2.58437100	-0.52676000	C	-3.96909100	-0.86059300	-0.24763200
H	4.15387900	1.47029100	-1.09355700	H	-4.98238500	-0.53563500	-0.46778700
H	2.98289100	-0.65135100	-1.37327400	H	-3.63905500	-1.52402600	-1.04693900
H	0.65285200	0.13502500	-1.94798900	H	-3.96834200	-1.40231200	0.70233700
H	0.51388700	3.47002900	0.04026000	C	0.15739600	-3.56752300	-0.23927100
H	2.91614900	3.51999400	-0.45147900	H	0.85628600	-4.37307300	-0.45763400
N	-1.01420000	1.34386200	-0.22630500	H	-0.29673400	-3.74982200	0.73919700
H	-1.46567500	2.21548400	0.02033800	H	-0.61157100	-3.55823500	-1.00978600
C	-1.77944500	0.18600800	-0.26802000	C	2.28076200	-2.42792200	0.27128000
C	-1.12230300	-1.05120700	-0.31256600	H	2.61686100	-1.48856600	0.69747100
C	0.26745700	-1.14463000	-0.39713200	H	2.25469300	-3.15867900	1.08073200
N	-3.10555300	0.32533100	-0.18528800	H	2.96441100	-2.78779200	-0.50055900
N	0.90762800	-2.30366800	-0.24897200	Cl	0.98961600	0.40361600	2.30604500

Cartesians coordinates for the optimized structure of $TS^{\ddagger}_{trans\text{-}5}$

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.487373; H = -1130.468663; G = -1130.532663)

atom	x	y	z	atom	x	y	z
C	2.84520100	1.98466800	-0.50253800	C	-4.00808000	1.24441500	0.08042500
C	2.26107300	0.87726700	-1.05344100	H	-4.49842700	1.24483700	1.06293400
C	0.84944900	0.65115600	-0.92799500	H	-3.41958700	2.14994900	-0.02375200
C	0.03767400	1.63382100	-0.25179500	H	-4.78537000	1.22398800	-0.68906400
C	0.67815200	2.80587000	0.25791200	C	-3.79856700	-1.20551600	0.03572500
C	2.03504900	2.96346900	0.14448300	H	-4.76652200	-1.14600400	-0.46675600
H	3.91380500	2.14561200	-0.58519300	H	-3.19682800	-1.97338700	-0.45088300
H	2.85409100	0.16167900	-1.61270900	H	-3.97517300	-1.50857200	1.07714600
H	0.36045000	0.16942300	-1.76365200	C	1.13950700	-0.59919000	2.28594400
H	0.06297700	3.55009100	0.75073700	H	1.21379800	-1.19848000	3.19598800
H	2.50705200	3.85003300	0.55472000	H	1.96704100	0.11979600	2.26799000
N	-1.26702800	1.44787100	-0.06425500	H	0.19605000	-0.06169800	2.29591500
C	-1.77092900	0.19139300	-0.02178600	C	2.47912700	-2.18393600	0.99381900
C	-0.99936900	-0.95685300	0.27707200	H	2.37404300	-3.09716900	0.41547300
C	0.39449000	-1.14211300	0.05853500	H	3.24162200	-1.54833900	0.52645300
N	-3.13833100	0.08428800	-0.06653900	H	2.81451600	-2.44483000	1.99774200
N	1.20066200	-1.48414400	1.11460200	Cl	0.83214800	-2.22900600	-1.45123400
H	-1.43383100	-1.66663600	0.97307500				

Cartesians coordinates for the optimized structure of $TS^{\ddagger}_{cis\text{-}5}$

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.525244; H = -1130.505251; G = -1130.576244)

atom	x	y	z	atom	x	y	z
C	2.26392400	2.74141700	-0.33153100	C	-4.23461400	0.60120700	0.65684000
C	1.60824000	2.01387100	-1.29757000	H	-5.06271000	0.70930000	-0.04738900
C	0.32738100	1.46293700	-1.03196100	H	-4.62213600	0.19419500	1.59624900
C	-0.30644700	1.71192000	0.22073900	H	-3.78381400	1.57015400	0.84592200
C	0.38507300	2.47911200	1.18912000	C	-3.70781400	-1.63597300	-0.25891600
C	1.64328500	2.96924900	0.91782600	H	-4.72452900	-1.54543300	-0.64220300
H	3.24163400	3.16270000	-0.53091900	H	-3.09345800	-2.07574200	-1.04304100
H	2.04623900	1.88463900	-2.28055600	H	-3.72316900	-2.30549400	0.60754200
H	-0.29621600	1.19330600	-1.87854000	C	1.08282300	-2.06719800	-2.67294800
H	-0.09568800	2.65571500	2.14306900	H	1.63142500	-1.56074400	-3.47003900
H	2.16650200	3.54402300	1.67333600	H	1.48157300	-3.07435900	-2.54292100
N	-1.53999300	1.22507600	0.50369600	H	0.02597100	-2.11379500	-2.92089800
C	-1.92956600	0.05618200	0.05832600	C	2.64084800	-1.12865600	-0.93993900
C	-0.94386400	-0.97073700	-0.33742500	H	2.63052800	-0.89365100	0.12180100
C	0.26706200	-0.75472200	-0.81606900	H	3.17998700	-2.06317600	-1.09200400
N	-3.23130600	-0.30117500	0.09504500	H	3.12034600	-0.33410700	-1.51582000
N	1.25910600	-1.32268400	-1.41007000	Cl	2.17798500	-2.29606900	2.62056200
H	-1.14085800	-1.99454500	-0.03280500				

Cartesians coordinates for the optimized structure of TS$^{‡}_{trans\text{-}5\cdot H}$

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.933357; H = -1130.915099; G = -1130.977488)

atom	x	y	z	atom	x	y	z
C	3.01806800	1.74830200	-0.54753800	H	-1.63578100	-1.92692100	-0.07943500
C	2.33602800	0.69601100	-1.09203800	C	-3.84821400	1.31246100	-0.64923500
C	0.91683000	0.53096400	-0.87998400	H	-4.11310200	0.91594000	-1.63766800
C	0.23599500	1.55239000	-0.11487900	H	-4.76196600	1.60201500	-0.12929400
C	0.95459500	2.63616100	0.41985900	H	-3.23376400	2.19847400	-0.79260400
C	2.31373500	2.72486700	0.19918200	C	-3.91503700	-0.91296700	0.37828400
H	4.08341200	1.85837400	-0.70309600	H	-4.92766800	-0.62506600	0.66020400
H	2.84205500	-0.02532200	-1.72189200	H	-3.97267500	-1.54832100	-0.51638700
H	0.36900700	0.22454200	-1.76717000	H	-3.47886500	-1.48860300	1.19496100
H	0.43746100	3.39396500	0.99619400	C	0.58998500	-0.73816800	2.31989400
H	2.85759600	3.56511600	0.61475200	H	-0.48913500	-0.61683300	2.32534800
N	-1.09634300	1.41824200	0.09421300	H	0.88130900	-1.33628400	3.18221000
H	-1.54854500	2.11591800	0.67216000	H	1.07085600	0.24533400	2.39574900
C	-1.77516700	0.17793100	0.01524000	C	2.41874400	-1.87221900	1.12104500
C	-1.09621400	-0.99225100	-0.05438700	H	2.56197700	-2.74090600	0.48440600
C	0.38500000	-1.13932900	-0.06896200	H	3.07974300	-1.06504300	0.77994800
N	-3.14024500	0.30165100	0.15060000	H	2.68298900	-2.13549600	2.14291400
N	1.02027700	-1.43683900	1.10342400	Cl	0.85901000	-2.29042200	-1.40105000

Cartesians coordinates for the optimized structure of TS$^{‡}_{cis\text{-}5\cdot H}$

(*in "dichloromethane", using the default polarizable continuum model*)

(E = -1130.935631; H = -1130.917030; G = -1130.980379)

atom	x	y	z	atom	x	y	z
C	-2.97237800	-1.81304900	-0.54781200	C	3.91156500	-1.18000400	-0.72462300
C	-2.34578400	-0.70453000	-1.03581200	H	4.25104300	-0.70361000	-1.65212000
C	-0.92440200	-0.50762100	-0.87018100	H	4.78330200	-1.51972600	-0.16393500
C	-0.17693400	-1.58434800	-0.26542400	H	3.30864500	-2.04441700	-0.99139100
C	-0.83435900	-2.74017000	0.19116900	C	3.88101400	0.98307500	0.44188000
C	-2.20165200	-2.83810500	0.06185700	H	4.90627300	0.70426100	0.68280100
H	-4.04169400	-1.94005600	-0.65563100	H	3.90292500	1.70644400	-0.38387300
H	-2.90688300	0.04467600	-1.57951100	H	3.43817000	1.45414200	1.31936400
H	-0.43066300	-0.04094400	-1.72073100	C	-0.50813300	2.85335200	-1.40640500
H	-0.26424000	-3.53391600	0.65866000	H	-0.82523800	2.36906700	-2.33903300
H	-2.70202200	-3.72445000	0.43396600	H	-0.90220300	3.86930600	-1.39364600
N	1.15755600	-1.42792600	-0.07551300	H	0.57664300	2.88630500	-1.38123200
H	1.63758600	-2.17395500	0.41266800	C	-2.45937200	2.42338000	0.00709100
C	1.78391500	-0.16668100	0.00164000	H	-3.02511700	2.35389500	-0.92682700
C	1.04147500	0.97247000	0.09075000	H	-2.87271300	1.73335000	0.73396900
C	-0.42320300	1.01342700	0.20084600	H	-2.55487500	3.44080600	0.39275400
N	3.14717000	-0.22881000	0.09372900	Cl	-1.01699900	0.56206500	1.93980500
N	-1.04266600	2.14044000	-0.24070600				
H	1.54511200	1.91062600	0.26463100				