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Supporting Information

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Using the Type II Cycloisomerization Reaction of 1,6-Enynes as a Mechanistic Probe to Identify the Real Catalytic Species of GaX₃ and InX₃

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1. Experimental Details

Anhydrous solvents (CH₃CN and DCE) were obtained by distillation after treating them with appropriate dehydration reagents. The reaction course was followed by TLC (petroleum ether–ethyl acetate) and GC analyses. Purification of resulting mixture involved concentration in vacuum and chromatographic separation by using silica gel. All NMR spectra were recorded on a 400 MHz spectrometer. ¹H and ¹³C NMR spectra were recorded using the deuterated solvent as the lock and the residual solvent as the internal reference. High-resolution mass spectra (HRMS) were performed under ESI ionization technique (using quadrupole analyzer). The compounds **1** and **2** have been reported in our previous work (Zhuo, L.-G.; Zhang, J.-J.; Yu, Z.-X. *J. Org. Chem.* **2012**, *77*, 8527.).

GaCl₃ catalyzed 1,6-enyne cycloisomerizations of **1 in DCE.** To a mixture of anhydrous DCE (2.5 mL) and GaCl₃ (10 mol %, 8.6 mg) under argon, 1,6-enyne (**1**, 0.50 mmol, 129 mg) was added. The resulting mixture was stirred at 80 °C for additional 1.5 h. The reaction was cooled to room temperature and the reaction mixture was directly concentrated in vacuum. The residue was subjected to flash column chromatography on silica gel (eluted with PE/EA 30:1 to 20:1) to give a mixture of diene products, **2**, 71 mg, 55% yield. The ratios of diene products were determined by NMR (*E*: *Z* = 2: 1).

InI₃ (75% yield of **2**, *E*: *Z* = 3: 1), InBr₃ (66% yield of **2**, *E*: *Z* = 3: 1) or GaBr₃ (56% yield of **2**, *E*: *Z* = 2: 1) catalyzed 1,6-enyne (**1**) cycloisomerization in DCE using similar procedure.

GaCl₃ catalyzed 1,6-enyne cycloisomerizations of **1 in CH₃CN.** To a mixture of anhydrous CH₃CN (1.5 mL) and GaCl₃ (53 mg, 0.30 mmol) under argon, **1** (60 mg, 0.25 mmol) and *n*-C₁₂H₂₆ (30 mg, internal standard) was added. The resulting mixture was stirred at room temperature overnight, and the GC determined conversion was 34% with *E*: *Z* = 2: 1 for **2**.

The starting mixture of GaCl₃ and **1** in CH₃CN was directly used for ESI-HRMS analysis.

HRMS (ESI), C₁₃H₁₈Cl₂GaO₄ (GaCl₂+**1**)⁺: calculated, 376.98325, found, 376.98382; GaCl₄, calculated, 208.80044, found, 208.80101.

InI₃, InBr₃ or GaBr₃ catalyzed 1,6-enyne (1**) cycloisomerization in CH₃CN using similar procedure.**

InBr₃ catalyzed reaction: 60% conversion, *E*: *Z* = 3: 1 for **2**

HRMS (ESI): C₁₃H₁₈Br₂InO₄ (InBr₂+**1**)⁺, calculated, 510.86048, found, 510.86151; InBr₄, calculated, 430.57666, found, 430.57681.

InI₃ catalyzed reaction: 50% conversion, *E*: *Z* = 3: 1 for **2**

HRMS (ESI): C₁₃H₁₈I₂InO₄ (InI₂+**1**)⁺, calculated, 606.83277, found, 606.83056; InI₄, calculated, 622.52120, found, 622.52030.

GaBr₃ catalyzed reaction: 44% conversion, *E*: *Z* = 3: 1 for **2**

HRMS (ESI): GaBr₄, calculated, 384.59948, found, 384.59864. The cationic complex (GaBr₂+**1**)⁺ was not detected.

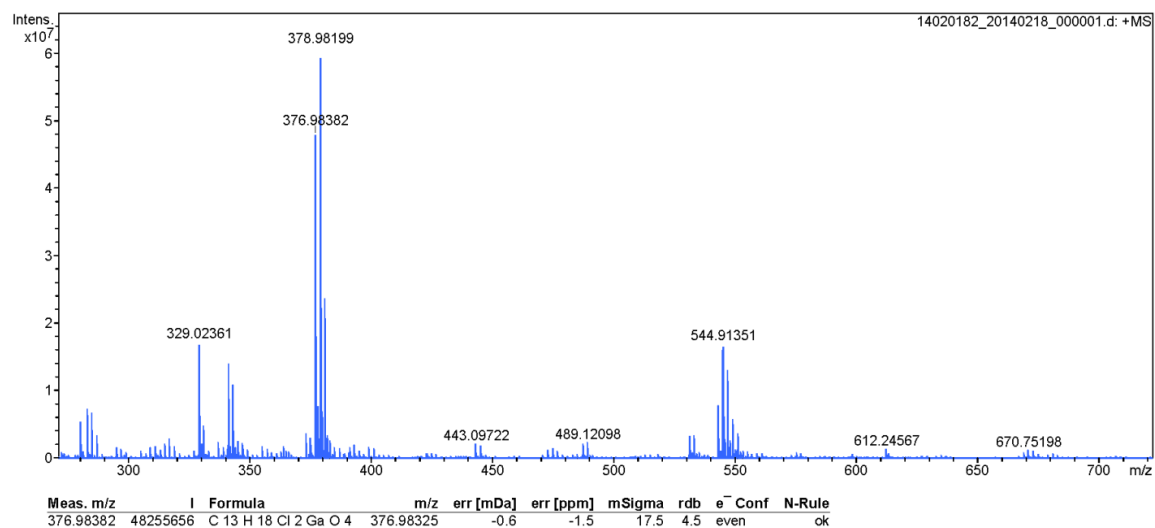
2. ESI-HRMS Spectra (GaCl₂+1)⁺

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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Sample I134-1
Comment ESI Positive

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Instrument Bruker Apex IV FTMS
Operator Peking University



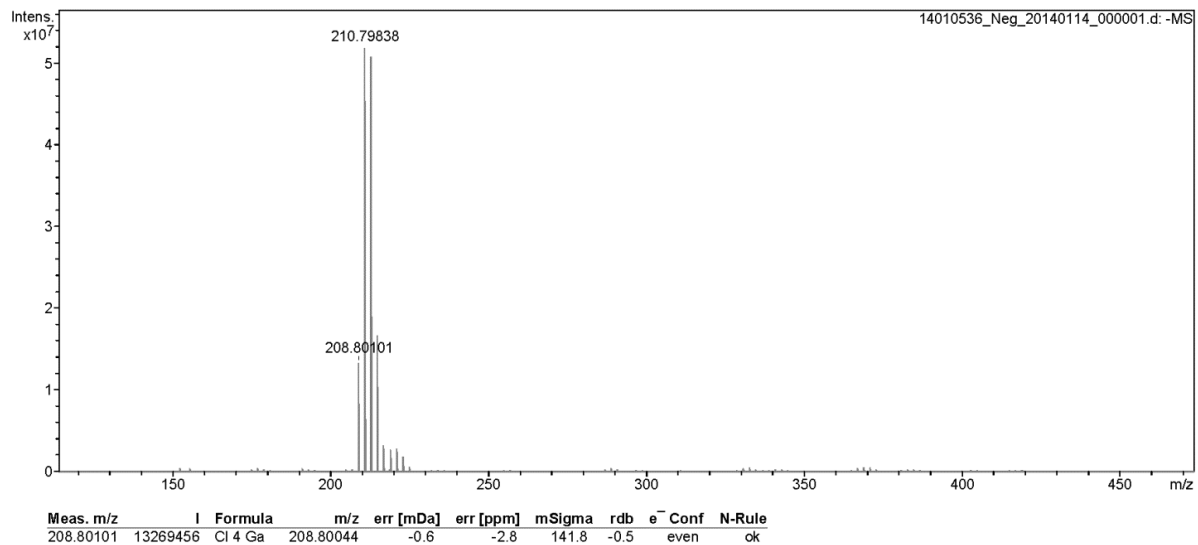


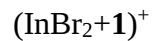
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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 Instrument Bruker Apex IV FTMS
 Operator Peking University



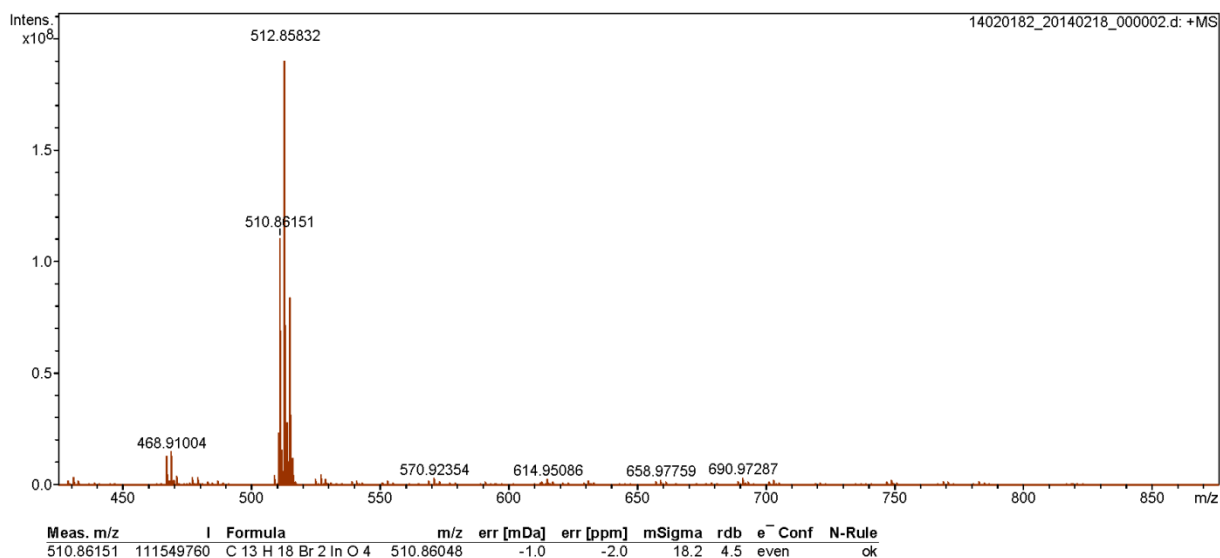


Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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 Instrument Bruker Apex IV FTMS
 Operator Peking University

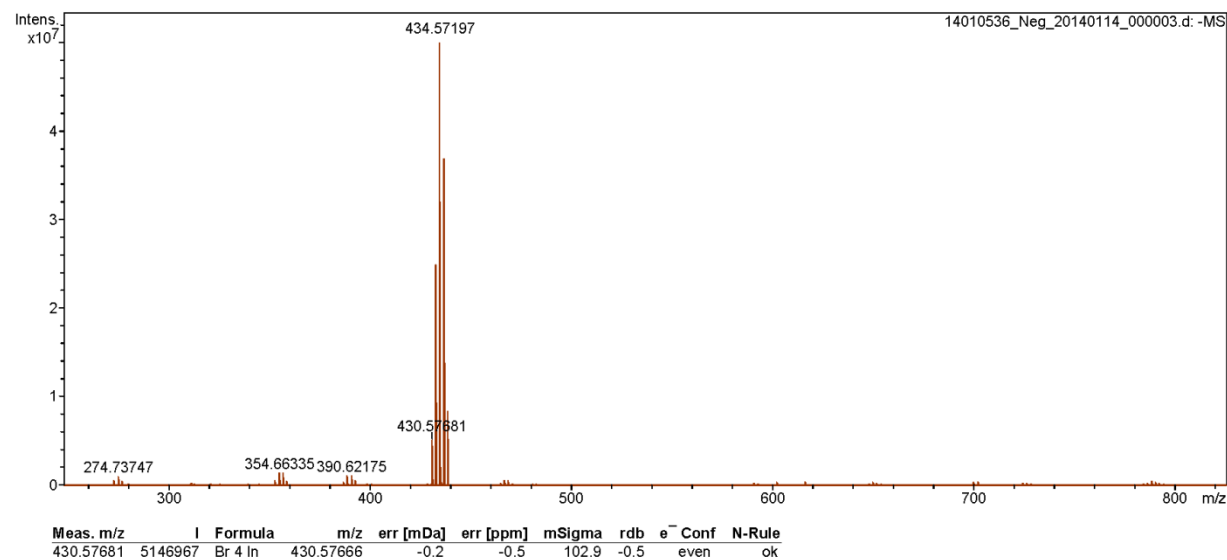


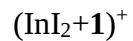


Peking University Mass Spectrometry Sample Analysis Report

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Comment	ESI Negative	Operator	Peking University



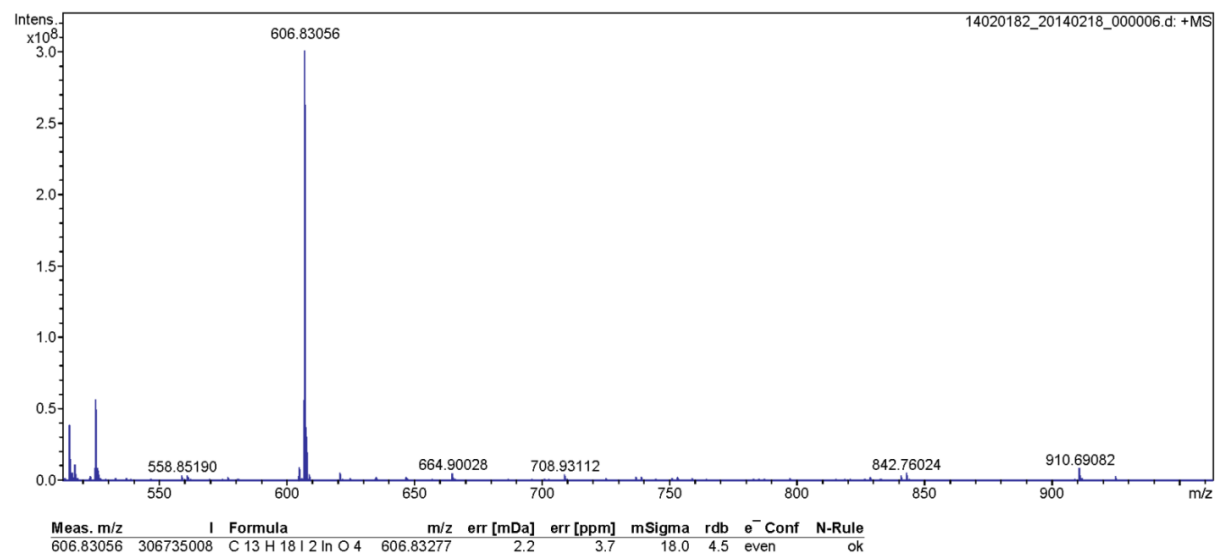


Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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 Sample I134-3
 Comment ESI Positive

Acquisition Date 2/18/2014 4:19:57 PM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



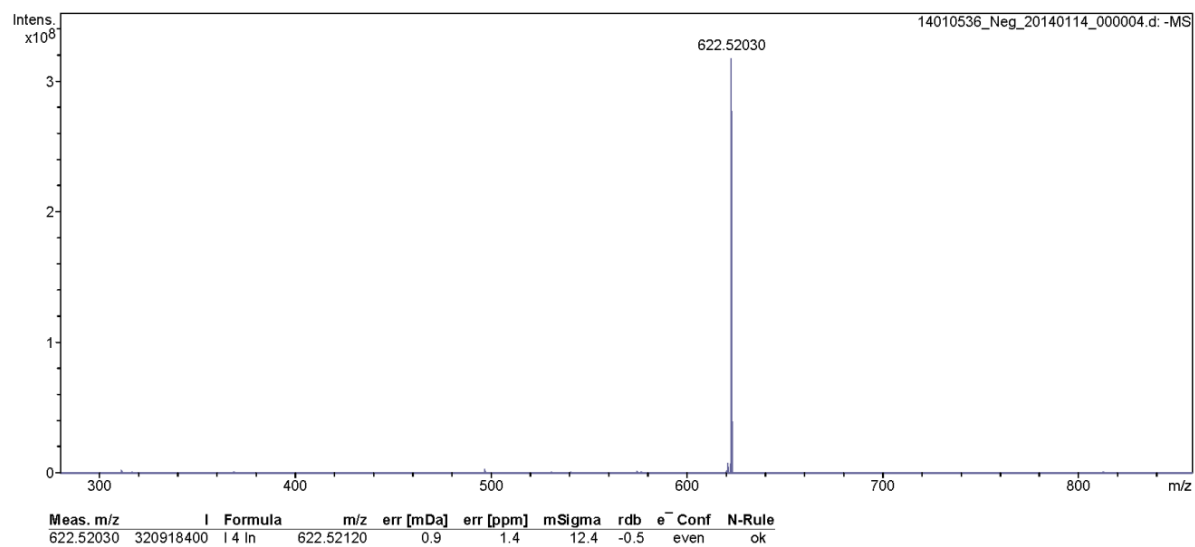
InL₄⁻

Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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Sample I134
Comment ESI Negative

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Instrument Bruker Apex IV FTMS
Operator Peking University



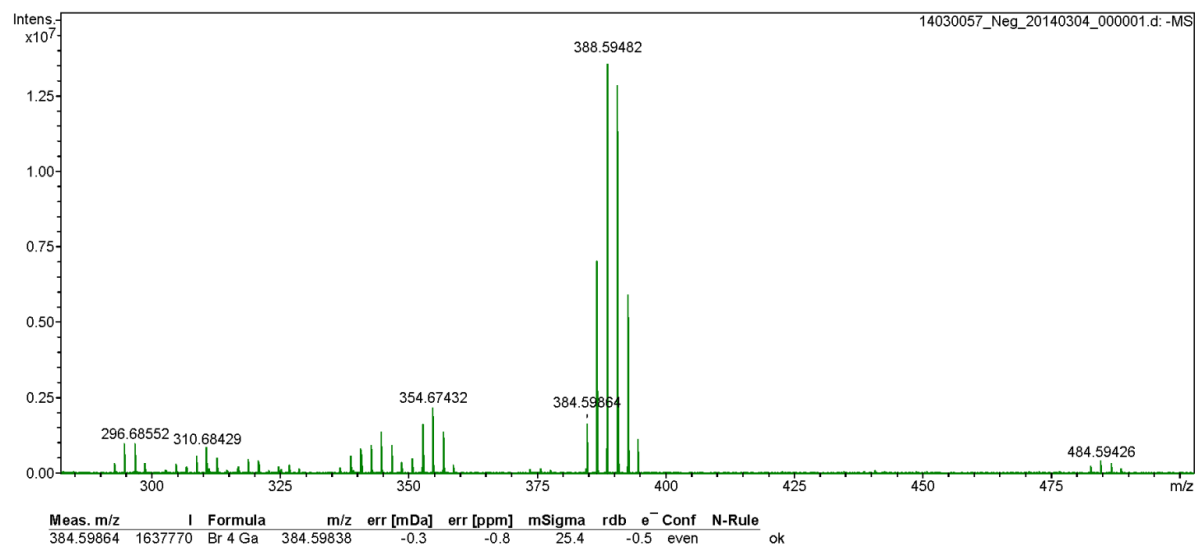


Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

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 Sample zlg-l137
 Comment ESI Negative

Acquisition Date 3/4/2014 3:41:05 PM
 Instrument Bruker Apex IV FTMS
 Operator Peking University



3. Computational Methods

All calculations were performed with the Gaussian 09 program.^[1] All gas phase stationary points were optimized using B3LYP functional^[2] with the LANL2DZ basis set^[3] and pseudo potential for the In, Ga, Br and I atoms, and the 6-31G(d) basis set^[4] for the other atoms (keyword 5D was used in the calculations). Full Hessian matrixes in Gaussian 09 were calculated to verify the nature of all stationary points as either minima or first-order saddle points. The first-order saddle points were further characterized by intrinsic reaction coordinate (IRC)^[5] calculations to confirm that the stationary points are correctly connected to the corresponding reactants and products. Solvation corrections to free energies were performed using UAHF radii and a CPCM^[6] dielectric continuum solvent model in 1,2-dichloroethane was used. Solvation calculations were carried out on the gas-phase optimized structures. All of the energies discussed in the paper and the Supporting Information are Gibbs free energies in gas phase at 298 K (ΔG_{gas}). Gibbs energies at 298 K in solution (ΔG_{sol}) (here the entropies were approximated by using the gas-phase computed entropies) and gas phase enthalpies (ΔH_{gas}) are also provided for reference. In our previous study, we have shown B3LYP is reliable in explain the experimentally observed regiochemistry.^[7]

[1] Full citation of Gaussian 09: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09*, Revision A. 02, Gaussian, Inc., Wallingford CT, 2009.

[2] (a) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648. (b) C. Lee, W. Yang, R.G. Parr, *Phys. Rev. B.* **1988**, 37, 785.

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[4] Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

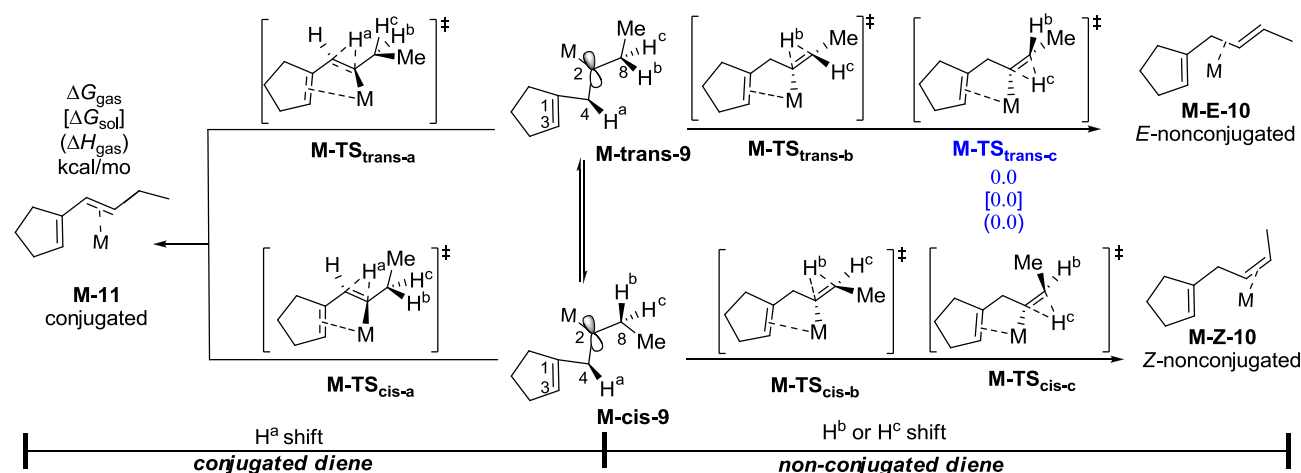
[5] (a) K. J. Fukui, *Phys. Chem.* **1970**, 74, 4161. (b) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.* **1989**, 90, 2154. (c) C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* **1990**, 94, 5523.

[6] (a) V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, 102, 1995. (b) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comput. Chem.* **2003**, 24, 669. (c) Y. Takano, K. N. Houk, *J. Chem. Theory. Comput.* **2005**, 1, 70.

[7] (a) L.-G. Zhuo, J.-J., Zhang, Z.-X., Yu, *J. Org. Chem.* **2012**, 77, 8527. (b) L.-G. Zhuo, J.-J., Zhang, Z.-X., Yu, *J. Org. Chem.* **2014**, in press (jo500059j).

4 Discussion of [1,2]H-shifts with Different Catalysts

We have only given the selected [1,2]-H shift transitions states in main text. Actually, intermediate **9** (named by **M-9** for different catalytic species, **M** = **GaCl₂⁺**, **GaCl₃**, (**GaCl₃**)₂, **InBr₂⁺**, **InBr₃**, **InI₂⁺**, **InI₃**, **GaBr₂⁺** or **GaBr₃**) have two conformers, one has the Me group and the C4 in the *trans* configuration, **M-trans-9**; another one has the **M-cis-9** with Me and C4 in *cis* conformation (not a minimum). H^b or H^c in **M-trans-9** could migrate to give *trans*-nonconjugated diene (**M-E-10**), via **M-TS_{trans-b}** or **M-TS_{trans-c}**, while the *cis*-nonconjugated diene product (**M-Z-10**) could be obtained from the H^b- or H^c-shift via **M-TS_{cis-b}** or **M-TS_{cis-c}**. All these transition states and their energies have been summarized in the following tables. All the energies are relative to the **M-TS_{trans-c}**.



M = **GaCl₂⁺**

	Name in text	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
GaCl₂-TS_{trans-a}		3.1	4.0	4.0
GaCl₂-TS_{cis-a}	TS_a	3.1	3.9	4.3
GaCl₂-TS_{trans-b}		0.6	1.3	0.9
GaCl₂-TS_{cis-b}		0.3	-0.1	0.4
GaCl₂-TS_{trans-c}	TS_{trans-c}	0.0	0.0	0.0
GaCl₂-TS_{cis-c}	TS_{cis-c}	0.5	0.5	0.6

M = **GaCl₃**

	Name in text	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
GaCl₃-TS_{trans-a}		-3.5	-2.9	-3.5
GaCl₃-TS_{cis-a}	GaCl₃-TS_a	-2.5	-2.4	-2.9
GaCl₃-TS_{trans-b}		-1.5	-2.5	-1.4
GaCl₃-TS_{cis-b}		-0.8	-1.3	0.3
GaCl₃-TS_{trans-c}		0.0	0.0	0.0
GaCl₃-TS_{cis-c}		-1.1	-2.7	-0.6

M = (GaCl₃)₂

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
(GaCl₃)₂-TS_{trans-a}	2.2	-1.4	-1.4
(GaCl₃)₂-TS_{cis-a}	2.6	-2.2	-1.2
(GaCl₃)₂-TS_{trans-b}	6.1	0.3	1.8
(GaCl₃)₂-TS_{cis-b}	4.2	-1.5	1.5
(GaCl₃)₂-TS_{trans-c}	2.5	-1.7	-0.8
(GaCl₃)₂-TS_{cis-c}	2.8	-0.5	-0.7

M = InBr₂⁺

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
InBr₂-TS_{trans-a}	2.2	1.6	2.8
InBr₂-TS_{cis-a}	2.4	1.9	3.4
InBr₂-TS_{trans-b}	-0.9	-1.5	-1.1
InBr₂-TS_{cis-b}	-0.5	-1.6	-0.6
InBr₂-TS_{trans-c}	0.0	0.0	0.0
InBr₂-TS_{cis-c}	-0.5	-1.3	-0.1

M = InBr₃

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
InBr₃-TS_{trans-a}	-0.7	0.3	-1.4
InBr₃-TS_{cis-a}	-0.6	-0.1	-1.0
InBr₃-TS_{trans-b}	0.3	0.2	0.2
InBr₃-TS_{cis-b}	0.3	0.5	1.3
InBr₃-TS_{trans-c}	0.0	0.0	0.0
InBr₃-TS_{cis-c}	0.8	-0.1	0.7

M = (InBr₃)₂

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
(InBr₃)₂-TS_{trans-a}	-0.5	0.4	-0.2
(InBr₃)₂-TS_{cis-a}	-0.1	1.0	-0.4
(InBr₃)₂-TS_{trans-b}	3.6	2.1	2.9
(InBr₃)₂-TS_{cis-b}	1.9	1.1	2.3
(InBr₃)₂-TS_{trans-c}	0.0	0.0	0.0
(InBr₃)₂-TS_{cis-c}	2.1	3.5	0.0

M = InI₂⁺

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
InI₂-TS_{trans-a}	1.8	1.8	2.3
InI₂-TS_{cis-a}	1.9	1.9	2.7
InI₂-TS_{trans-b}	-0.6	-1.3	-1.0
InI₂-TS_{cis-b}	-0.4	-1.4	-0.7
InI₂-TS_{trans-c}	0.0	0.0	0.0
InI₂-TS_{cis-c}	-0.2	-0.7	0.0

M = InI₃

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
InI₃-TS_{trans-a}	-3.5	-3.2	-3.6
InI₃-TS_{cis-a}	-2.8	-2.9	-3.1
InI₃-TS_{trans-b}	-1.8	-2.7	-1.7
InI₃-TS_{cis-b}	-0.2	-1.0	0.3
InI₃-TS_{trans-c}	0.0	0.0	0.0
InI₃-TS_{cis-c}	-1.7	-3.3	-1.3

M = (InI₃)₂

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
(InI₃)₂-TS_{trans-a}	-0.5	0.7	-0.4
(InI₃)₂-TS_{cis-a}	0.6	0.8	-0.1
(InI₃)₂-TS_{trans-b}	3.6	2.5	3.0
(InI₃)₂-TS_{cis-b}	1.8	1.1	2.1
(InI₃)₂-TS_{trans-c}	0.0	0.0	0.0
(InI₃)₂-TS_{cis-c}	1.0	1.2	1.6

M = GaBr₂⁺

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
GaBr₂-TS_{trans-a}	2.4	3.0	3.1
GaBr₂-TS_{cis-a}	2.1	2.7	3.2
GaBr₂-TS_{trans-b}	-0.8	-1.6	-1.0
GaBr₂-TS_{cis-b}	-0.7	-1.7	-0.7
GaBr₂-TS_{trans-c}	0.0	0.0	0.0
GaBr₂-TS_{cis-c}	-0.3	-1.2	0.1

M = GaBr₃

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
GaBr₃-TS_{trans-a}	-0.7	0.5	-1.4
GaBr₃-TS_{cis-a}	-0.2	0.6	-1.0
GaBr₃-TS_{trans-b}	1.0	0.6	0.4
GaBr₃-TS_{cis-b}	1.0	1.1	1.0
GaBr₃-TS_{trans-c}	0.0	0.0	0.0
GaBr₃-TS_{cis-c}	1.5	0.4	1.2

M = (GaBr₃)₂

	ΔG_{gas}	ΔG_{sol}	ΔH_{gas}
(GaBr₃)₂-TS_{trans-a}	2.2	-1.4	-1.4
(GaBr₃)₂-TS_{cis-a}	2.6	-2.2	-1.2
(GaBr₃)₂-TS_{trans-b}	6.1	0.3	1.8
(GaBr₃)₂-TS_{cis-b}	4.2	-1.5	1.5
(GaBr₃)₂-TS_{trans-c}	2.5	-1.7	-0.8
(GaBr₃)₂-TS_{cis-c}	2.8	-0.5	-0.7

5. Computed Energies of All Stationary Points

thermal enthalpy (H , in Hartree)

thermal free energy (G , in Hartree)

thermal correction to Gibbs free energy ($TCGFE$, in Hartree)

total free energy in solution (E_{sol} , in hartree),

thermal corrected Gibbs free energy in dichloroethane solution (G_{sol} , which equals to $E_{sol} + TCGFE$, in Hartree).

	$TCGFE$	H	G	G_{sol}	E_{sol}
GaCl₂-TS_{trans-a}	0.163206	-1273.390868	-1273.451118	-1273.551195	-1273.714401
TS_a	0.162404	-1273.390506	-1273.451145	-1273.551296	-1273.713700
GaCl₂-TS_{trans-b}	0.163721	-1273.395823	-1273.455180	-1273.555514	-1273.719235
GaCl₂-TS_{cis-b}	0.163844	-1273.396607	-1273.455666	-1273.557805	-1273.721649
TS_{trans-c}	0.163972	-1273.397308	-1273.456098	-1273.557581	-1273.721553
TS_{cis-c}	0.163313	-1273.396431	-1273.455224	-1273.556755	-1273.720068
GaCl₃-TS_{trans-a}	0.162026	-1733.884615	-1733.949322	-1733.967897	-1734.129923
GaCl₃-TS_{cis-a}	0.162351	-1733.883698	-1733.947762	-1733.967036	-1734.129387
GaCl₃-TS_{trans-b}	0.161144	-1733.881292	-1733.946206	-1733.967350	-1734.128494
GaCl₃-TS_{cis-b}	0.159956	-1733.878593	-1733.945089	-1733.965439	-1734.125395
GaCl₃-TS_{trans-c}	0.161694	-1733.879081	-1733.943741	-1733.963288	-1734.124982
GaCl₃-TS_{cis-c}	0.160666	-1733.879982	-1733.945424	-1733.967544	-1734.128210
(GaCl₃)₂-TS_{trans-a}	0.154233	-3116.695037	-3116.779930	-3116.810035	-3116.964268
(GaCl₃)₂-TS_{cis-a}	0.154310	-3116.694854	-3116.779221	-3116.811223	-3116.965533
(GaCl₃)₂-TS_{trans-b}	0.154583	-3116.690027	-3116.773584	-3116.807338	-3116.961921
(GaCl₃)₂-TS_{cis-b}	0.152051	-3116.690405	-3116.776682	-3116.810214	-3116.962265
(GaCl₃)₂-TS_{trans-c}	0.153004	-3116.694128	-3116.779322	-3116.810466	-3116.963470
(GaCl₃)₂-TS_{cis-c}	0.153623	-3116.693922	-3116.778914	-3116.808612	-3116.962235
InBr₂-TS_{trans-a}	0.157827	-379.15106	-379.21588	-379.32131	-379.47913
InBr₂-TS_{cis-a}	0.156835	-379.150047	-379.215564	-379.32089	-379.477726
InBr₂-TS_{trans-b}	0.158653	-379.157278	-379.220723	-379.32635	-379.485008
InBr₂-TS_{cis-b}	0.158512	-379.156439	-379.220183	-379.32639	-379.484902
InBr₂-TS_{trans-c}	0.158568	-379.155494	-379.21935	-379.3239	-379.482464
InBr₂-TS_{cis-c}	0.157836	-379.155729	-379.220194	-379.326	-379.483834
InBr₃-TS_{trans-a}	0.152837	-387.262360	-387.335309	-387.354073	-387.506910
InBr₃-TS_{cis-a}	0.151936	-387.261661	-387.335093	-387.354709	-387.506645
InBr₃-TS_{trans-b}	0.151213	-387.259751	-387.333596	-387.354220	-387.505433
InBr₃-TS_{cis-b}	0.149755	-387.258068	-387.333725	-387.353668	-387.503423
InBr₃-TS_{trans-c}	0.151119	-387.260139	-387.334143	-387.354537	-387.505656
InBr₃-TS_{cis-c}	0.151272	-387.258946	-387.332930	-387.354641	-387.505913
(InBr₃)₂-TS_{trans-a}	0.139588	-434.163661	-434.261573	-434.285491	-434.425079
(InBr₃)₂-TS_{cis-a}	0.140168	-434.164091	-434.260995	-434.284539	-434.424707
(InBr₃)₂-TS_{trans-b}	0.140346	-434.158799	-434.255106	-434.282751	-434.423097
(InBr₃)₂-TS_{cis-b}	0.138730	-434.159727	-434.257847	-434.284309	-434.423039
(InBr₃)₂-TS_{trans-c}	0.139325	-434.163412	-434.260828	-434.286091	-434.425416

(InBr₃)₂-TS_{cis-c}	0.142163	-434.163487	-434.257505	-434.280562	-434.422725
InI₂-TS_{trans-a}	0.155898	-375.587405	-375.654132	-375.754333	-375.910231
InI₂-TS_{cis-a}	0.155213	-375.586909	-375.653981	-375.754151	-375.909364
InI₂-TS_{trans-b}	0.156772	-375.592802	-375.658012	-375.759259	-375.916031
InI₂-TS_{cis-b}	0.156622	-375.592198	-375.657711	-375.759409	-375.916031
InI₂-TS_{trans-c}	0.156404	-375.591149	-375.657019	-375.757177	-375.913581
InI₂-TS_{cis-c}	0.156142	-375.591144	-375.657274	-375.758227	-375.914369
InI₃-TS_{trans-a}	0.154981	-392.616466	-392.687451	-392.708590	0.154981
InI₃-TS_{cis-a}	0.154847	-392.615631	-392.686336	-392.708250	0.154847
InI₃-TS_{trans-b}	0.153957	-392.613410	-392.684723	-392.707808	0.153957
InI₃-TS_{cis-b}	0.153735	-392.610257	-392.682298	-392.705209	0.153735
InI₃-TS_{trans-c}	0.154228	-392.610681	-392.681925	-392.703548	0.154228
InI₃-TS_{cis-c}	0.153413	-392.612681	-392.684602	-392.708773	0.153413
(InI₃)₂-TS_{trans-a}	0.134193	-423.455338	-423.558275	-423.579666	-423.713859
(InI₃)₂-TS_{cis-a}	0.134093	-423.455000	-423.556570	-423.579584	-423.713677
(InI₃)₂-TS_{trans-b}	0.134515	-423.449961	-423.551751	-423.576908	-423.711423
(InI₃)₂-TS_{cis-b}	0.133294	-423.451431	-423.554690	-423.579121	-423.712415
(InI₃)₂-TS_{trans-c}	0.133588	-423.454764	-423.557538	-423.580830	-423.714418
(InI₃)₂-TS_{cis-c}	0.133488	-423.452270	-423.556000	-423.578927	-423.712415
GaBr₂-TS_{trans-a}	0.160146	-379.329713	-379.392698	-379.493894	-379.654040
GaBr₂-TS_{cis-a}	0.159132	-379.329569	-379.393088	-379.494393	-379.653525
GaBr₂-TS_{trans-b}	0.160887	-379.336221	-379.397754	-379.501237	-379.662124
GaBr₂-TS_{cis-b}	0.160709	-379.335729	-379.397540	-379.501446	-379.662155
GaBr₂-TS_{trans-c}	0.160925	-379.334657	-379.396499	-379.498738	-379.659663
GaBr₂-TS_{cis-c}	0.160187	-379.334564	-379.397027	-379.500594	-379.660781
GaBr₃-TS_{trans-a}	0.157785	-392.793705	-392.862266	-392.881750	-393.039535
GaBr₃-TS_{cis-a}	0.157512	-392.793049	-392.861452	-392.881683	-393.039195
GaBr₃-TS_{trans-b}	0.156761	-392.790795	-392.859646	-392.881539	-393.038300
GaBr₃-TS_{cis-b}	0.156221	-392.789852	-392.859540	-392.880751	-393.036972
GaBr₃-TS_{trans-c}	0.155781	-392.791430	-392.861175	-392.882563	-393.038344
GaBr₃-TS_{cis-c}	0.156494	-392.789592	-392.858861	-392.881990	-393.038484
(GaBr₃)₂-TS_{trans-a}	0.143385	-434.508520	-434.603085	-434.621992	-434.765377
(GaBr₃)₂-TS_{cis-a}	0.144356	-434.508716	-434.601963	-434.620777	-434.765133
(GaBr₃)₂-TS_{trans-b}	0.144384	-434.502861	-434.595558	-434.618081	-434.762465
(GaBr₃)₂-TS_{cis-b}	0.143223	-434.504224	-434.598343	-434.620850	-434.764073
(GaBr₃)₂-TS_{trans-c}	0.143756	-434.507822	-434.601225	-434.621782	-434.765538
(GaBr₃)₂-TS_{cis-c}	0.143451	-434.507971	-434.602115	-434.621054	-434.764505
	0.143385	-434.508520	-434.603085	-434.621992	-434.765377
4	0.165261	-1273.408930	-1273.470828	-1273.560568	-1273.725829
5	0.210229	-2272.360890	-2272.444124	-2272.534284	-2272.744513
6	0.211302	-2272.352048	-2272.433260	-2272.516176	-2272.727478
TS1	0.213362	-2272.350571	-2272.429181	-2272.514102	-2272.727464

7	0.217907	-2272.370933	-2272.447454	-2272.534678	-2272.752585
TS2	0.218983	-2272.363879	-2272.437843	-2272.531526	-2272.750509
8	0.216126	-2272.370001	-2272.447146	-2272.538986	-2272.755112
9	0.166871	-1273.404401	-1273.464352	-1273.559991	-1273.726862
DCE	0.030296	-998.946334	-998.980535	-998.988962	-999.019258
E-10	0.168657	-1273.445970	-1273.505142	-1273.603205	-1273.771862
Z-10	0.169084	-1273.443823	-1273.502743	-1273.601513	-1273.770597
11	0.165008	-1273.433749	-1273.496389	-1273.587114	-1273.752122
GaCl₃-9	0.167139	-1733.898497	-1733.961626	-1733.997624	-1734.164763

6. Coordinates of All Stationary Points

GaCl₂-TS_{trans-a}

H	0.00250900	1.42427100	-1.58032700
C	-0.36161600	1.91860500	-0.46567300
C	0.90092000	1.29027600	-0.54683500
C	-2.82958700	-0.08084600	1.57394600
C	-3.62618000	0.04433400	0.24920000
C	-1.52368400	1.17811600	0.05330000
C	-1.48687800	0.50472800	1.23295300
H	-0.45856600	2.99228300	-0.66501900
C	-2.91094300	1.16009100	-0.55934300
H	-0.65151300	0.51553600	1.93279100
H	-2.75840300	-1.10873600	1.94698900
H	-3.27320300	0.51022400	2.38867500
H	-3.56852100	-0.89795500	-0.30407300
H	-4.68236900	0.26565400	0.41414600
H	-3.38417200	2.14268000	-0.41749900
H	-2.90017200	0.96523800	-1.63728500
Cl	-0.15651200	-1.84005400	-1.76494900
Cl	1.69481600	-1.56114600	1.50666700
C	2.16483200	2.05330000	-0.79552100
C	2.92045100	2.19792200	0.55448700
H	1.95211900	3.04861000	-1.20459600
H	2.80141100	1.51683000	-1.50694900
H	3.85171900	2.73924800	0.36754200
H	2.33324600	2.76685600	1.28140600
H	3.17446000	1.22681700	0.98918900
Ga	0.70730300	-0.70601000	-0.17397700

TS_a

H	-0.24416200	1.61730200	1.12691000
C	0.25660100	1.85313600	-0.01443000
C	-1.00087400	1.21132200	0.04301400
C	2.98174900	-0.51555100	-1.14233800
C	3.80554700	0.40332700	-0.19576500
C	1.48931000	1.06698800	-0.19741800
C	1.61266500	0.10863200	-1.15026200
H	0.32101200	2.94434600	-0.06294100
C	2.76727700	1.24802500	0.59515500
H	0.86698100	-0.11830000	-1.91281700
H	2.91673000	-1.54896100	-0.77185700
H	3.40110400	-0.57939300	-2.15199800
H	4.45697700	-0.16696700	0.46929500
H	4.44384800	1.06397200	-0.78918000
H	3.05161300	2.30382800	0.68013800
H	2.62543000	0.87982300	1.62105400
Cl	-0.06075200	-1.59359300	2.00268600
Cl	-1.63504600	-1.97045600	-1.41190500
C	-2.31154600	1.93216400	-0.03989100
C	-2.29829500	3.46343100	-0.01193700
H	-2.99242200	1.52500100	0.71937600
H	-2.73131400	1.56963200	-0.99627000
H	-3.32273800	3.83404500	-0.10124600
H	-1.89403400	3.84949800	0.93092200
H	-1.72306500	3.88636100	-0.84211400
Ga	-0.77941900	-0.80968400	0.15228000

GaCl₂-TS_{trans-b}

H	-2.05246700	1.75385600	1.13814800
C	-1.07669400	1.36044400	0.14472100
C	-2.34297200	1.93963400	-0.04051000
C	2.55636700	-0.21403300	-1.61191100
C	3.34220200	-0.02027400	-0.28777700
C	0.19578900	2.17170300	0.27074500
C	1.32939900	1.30087500	-0.24347400
H	0.14440800	3.13423900	-0.25687600
H	0.37425400	2.39704100	1.33158800
H	0.44583000	0.53800700	-2.08348900
H	2.42281500	-1.26405900	-1.89052500
H	3.05094700	0.27381200	-2.46372900
H	3.22202300	-0.90326900	0.34804700
H	4.41186700	0.11964600	-0.45530300
H	3.23374600	2.13741800	0.19659700
H	2.63263700	1.10841800	1.49545700
Cl	0.30866900	-1.14029800	2.13824400
Cl	-1.27769600	-2.01157100	-1.16119200
C	1.25181100	0.50273800	-1.34879800
C	-3.60552800	1.17711700	-0.36182100
H	-2.39006000	3.02587500	-0.17516000
C	2.68900400	1.20368800	0.40561500
H	-4.46175100	1.59041300	0.17828400

H	-3.80444100	1.30024500	-1.43352400
H	-3.51719300	0.10875000	-0.15082500
Ga	-0.42824000	-0.58935300	0.19518300

GaCl₂-TS_{cis-b}

H	2.25847200	-0.54585800	-1.12944500
C	1.51387600	-0.69711800	0.04873000
C	2.91122300	-0.70798600	-0.06900800
C	-2.62135700	-0.55323300	-1.41792600
C	-3.13692800	-1.14011500	-0.07762100
C	0.64715200	-1.93252300	0.07261700
C	-0.77532800	-1.55466100	-0.29373100
H	1.02257300	-2.76190500	-0.54252300
H	0.68415600	-2.29401600	1.11324200
H	-0.44088700	-0.36476300	-2.08937500
H	-2.94032900	0.47895800	-1.59269700
H	-2.96352400	-1.13699600	-2.28391300
H	-2.15608700	-3.11141100	0.13476400
H	-1.88136700	-2.05615300	1.51872000
Cl	0.48442200	2.49297300	-1.19997400
Cl	-0.63547700	1.09704500	2.12742200
C	-1.11937300	-0.70371300	-1.30453500
C	3.82075000	-1.90648900	-0.05975300
H	3.40309900	0.26516800	0.01154200
C	-1.99810500	-2.06196400	0.42925800
H	4.25401800	-1.97840200	0.94688100
H	3.30689400	-2.84490400	-0.27803800
H	4.65127500	-1.77066800	-0.75813400
H	-4.08388000	-1.67140400	-0.19064900
H	-3.29568200	-0.33281100	0.64427500
Ga	0.17089500	0.85940900	0.15356600

TS_{trans-c}

H	-1.69935100	1.53335700	-1.20325700
C	-1.07479700	1.36667200	-0.00823100
C	-2.33294200	1.95531900	-0.17644600
C	2.69577500	-0.37348800	-1.40841300
C	3.40009200	-0.01115500	-0.07460200
C	0.20770700	2.16672300	0.06295200
C	1.37655900	1.27309400	-0.30190500
H	0.19312900	3.09598600	-0.52431700
H	0.29593800	2.47691500	1.11609700
H	0.60686400	0.27482000	-2.08109200
H	2.59634000	-1.45127800	-1.57026600
H	3.23197100	0.02587800	-2.28064600
H	3.23841800	-0.80795800	0.65841100
H	4.47828200	0.11410000	-0.19143200
H	3.25043400	2.18792700	0.10504500
C	2.59752400	1.33990000	1.50460300
Cl	-1.30499000	-2.03018400	-1.16454300
Cl	0.18358500	-1.05196100	2.16183200
C	1.36525100	0.33995100	-1.29882500
C	-3.64610200	1.23430600	-0.07226300
C	2.70342300	1.28384100	0.41553400
H	-2.38073100	3.04659400	-0.26628800
H	-3.53655200	0.14850000	-0.13210100
H	-4.07552800	1.48854700	0.90645800
H	-4.35105600	1.57990300	-0.83366900
Ga	-0.43714900	-0.58284800	0.16166900

TS_{cis-c}

H	2.49358900	-0.51159700	1.15430400
C	1.53660600	-0.64413400	0.09439200
C	2.93758800	-0.59441700	0.00295400
C	-2.53107700	-0.68100900	-1.47238300
C	-3.06927700	-1.20655900	-0.11526300
C	0.72887300	-1.92564200	0.14708100
C	-0.69625300	-1.58748400	-0.25309100
H	1.14965500	-2.70493800	-0.50319100
H	0.74203800	-2.32932300	1.16898200
H	-0.33473100	-0.49321400	-2.10121700
H	-2.86391300	0.33420700	-1.70971000
H	-2.84056900	-1.31553200	-2.31476100
H	-3.26389100	-0.36561600	0.55779700
H	-4.00174300	-1.76375000	-0.22394400
H	-2.05688600	-3.14310900	0.23299000
H	-1.83751200	-2.00475000	1.56041400
Cl	-0.70856800	1.09841400	2.10354700
Cl	0.35720900	2.48882400	-1.23117500
C	-1.03041700	-0.79911300	-1.31789200

C	3.88042500	-1.75195300	-0.20801600
C	-1.92678600	-2.07560200	0.47082400
H	3.36849500	0.40207400	-0.12690100
H	4.80042900	-1.60833400	0.36604700
H	3.44410500	-2.71876500	0.05118100
H	4.16222300	-1.76523200	-1.26876700
Ga	0.13012000	0.85807400	0.13660700

GaCl₃-TS_{trans-a}

H	-0.53633900	1.17525700	-1.54640800
C	-1.12174000	1.59146200	-0.53570800
C	0.26472600	1.33295300	-0.38247900
C	-3.66584600	-0.80674200	0.92001300
C	-4.55432500	0.02101900	-0.04589400
C	-2.26240900	0.73194400	-0.18967100
C	-2.32803300	-0.12396400	0.84560000
H	-1.39418800	2.62416700	-0.79541600
C	-3.56224800	0.76582100	-0.97604700
H	-1.52111500	-0.32550300	1.54298600
H	-3.55096400	-1.84879200	0.58543800
H	-4.06294200	-0.85114300	1.94068700
H	-5.26468700	-0.59740500	-0.60102800
H	-5.13518600	0.75098100	0.52869300
H	-3.89190700	1.78502400	-1.21741100
H	-3.43373000	0.24239100	-1.93479400
Cl	-0.03034400	-1.98288700	-1.25249000
Cl	3.19882200	-0.34526100	-0.77513000
Cl	1.05305900	-0.87745000	2.13317700
C	1.19237000	2.50482600	-0.54071300
C	1.68289200	2.91773100	0.87087300
H	0.69186700	3.35917100	-1.01721100
H	2.06212500	2.22045600	-1.14015800
H	2.36500400	3.76711700	0.77005400
H	0.84844200	3.21777400	1.51309000
H	2.22172400	2.10298600	1.36162900
Ga	1.12785300	-0.53992300	-0.05098300

GaCl₃-TS_{cis-a}

H	-0.44268200	1.47656400	-1.10958000
C	-1.09347700	1.58904400	-0.04819900
C	0.29338200	1.32502600	0.07567100
C	-3.58747600	-1.17701100	0.62659900
C	-4.46567000	-0.17189000	-0.16533000
C	-2.20628300	0.63099200	0.00073100
C	-2.28123600	-0.45105200	0.79560900
H	-1.40462300	2.63954400	-0.03255200
C	-3.46558800	0.80885400	-0.82994700
H	-1.50039300	-0.78604300	1.47107900
H	-3.40640400	-2.10345400	0.06107000
H	-4.03197800	-1.47846700	1.58207800
H	-5.11717500	-0.66255000	-0.89337900
H	-5.10824300	0.37749000	0.53156100
H	-3.83138000	1.84417000	-0.84126400
H	-3.26356900	0.53518600	-1.87583800
Cl	0.06416800	-1.72395600	-1.56488700
Cl	3.25046900	-0.18387200	-0.70686100
Cl	1.09537900	-1.36080800	2.00427100
C	1.24530700	2.47432100	0.27830600
C	0.72482400	3.91387400	0.24023400
H	2.09866100	2.34249900	-0.39725200
H	1.67264200	2.25433300	1.27256100
H	1.55399600	4.60221000	0.42914500
H	0.30638300	4.17292200	-0.74001100
H	-0.03944600	4.10395800	1.00205200
Ga	1.17939400	-0.56143500	-0.05660000

GaCl₃-TS_{trans-b}

H	0.89987900	1.42248600	-1.68208300
C	0.07072500	0.96149500	-0.88067800
C	0.31788700	2.33388900	-0.76642400
C	-3.65832300	0.20178200	1.33302100
C	-4.54801700	-0.20239900	0.12827800
C	-1.19804600	0.54445600	-1.59993000
C	-2.32196500	0.31603600	-0.61718900
H	-1.50497100	1.29470600	-2.34794000
H	-1.01431400	-0.38909100	-2.14517500
H	-1.58839100	1.15239500	1.23823700
H	-3.45149800	-0.65166000	1.99506700
H	-4.12114100	0.97458100	1.95919300

H	-5.17829000	-1.07107100	0.33931300
H	-5.21358900	0.62964500	-0.12840600
H	-3.95877800	-0.11850200	-2.00835400
H	-3.31394300	-1.51645100	-1.15208600
Cl	0.36718300	-2.43614800	-0.39599200
Cl	3.23186500	-0.16258100	-0.78799700
Cl	1.17841800	0.03862700	2.24582800
C	-2.37918800	0.66396700	0.67600300
C	1.42276600	2.98570700	-0.00436900
H	-0.37662900	3.01492400	-1.27428200
C	-3.56142200	-0.45062000	-1.03974400
H	1.81215500	3.85944500	-0.53546400
H	0.97980200	3.34150000	0.93773300
H	2.23240100	2.29878400	0.24756200
Ga	1.21657700	-0.47889800	0.10102000

GaCl₃-TS_{cis-b}

H	-0.37963600	1.23652000	0.88723200
C	0.16936300	2.35076800	0.24524300
C	-0.04045900	1.08531000	-0.31045700
C	-4.53025600	-0.14918300	0.45055500
C	-3.84503900	-1.53903700	0.34313100
C	-1.22408200	0.82011800	-1.23494300
C	-3.57541600	0.75879800	-0.28768900
H	-1.55238200	1.74121200	-1.72967400
H	-0.85204300	0.14607400	-2.01724000
H	-3.83250700	1.77804000	-0.56972900
H	-4.64081300	0.17529000	1.49670200
H	-5.53911200	-0.14330900	0.01967000
H	-3.95985400	-2.13719000	1.25147300
H	-4.30001400	-2.10387900	-0.47778800
H	-1.94302100	-1.95587000	-0.72125400
H	-1.71604200	-1.31869300	0.89515400
Cl	1.25844400	-1.84028100	-1.58307300
Cl	3.32746100	0.81716800	-0.04384400
Cl	1.03767400	-1.09404200	2.05520700
C	-2.39608700	0.17145400	-0.53101700
C	-0.63216900	3.60064900	0.06577100
H	1.05653200	2.45305500	0.87632300
C	-2.35897400	-1.24862700	0.00624300
H	-0.75100900	4.12486900	1.01926400
H	-0.04776500	4.26287900	-0.58951200
H	-1.60821500	3.43281400	-0.38992700
Ga	1.45367000	-0.34844200	0.00926900

GaCl₃-TS_{trans-c}

H	-0.50377500	1.38519000	0.54419900
C	-0.08804300	0.98767000	-0.56096300
C	0.05708300	2.35290900	-0.30031600
C	-4.67842800	0.38322000	0.30645000
C	-4.09634600	-1.01023900	0.66994600
C	-1.27186800	0.57049900	-1.44180200
C	-2.50905700	0.23898600	-0.64006500
H	-1.49973700	1.36898500	-2.16000700
H	-0.95377500	-0.31047600	-2.01221600
H	-3.81291000	1.85085200	-1.22364200
H	-4.79000000	1.02759800	1.19206300
H	-5.67389800	0.31599600	-0.14966700
H	-4.26599700	-1.27875300	1.71650800
H	-4.58166400	-1.77668800	0.05621600
H	-2.22072300	-1.86942200	-0.14966700
H	-1.95974300	-0.78264500	1.19755600
Cl	0.79409100	-2.33367700	-0.85875800
Cl	3.26397200	0.37363600	-0.77496200
Cl	1.26270700	-0.34739700	2.23495300
C	-3.64344000	0.95166400	-0.63486800
C	1.15350100	3.01330900	0.46956800
C	-2.58887900	-0.94465600	0.30872200
H	-0.70269900	3.02725200	-0.71558800
H	0.77252500	3.85195500	1.06010200
H	1.71001000	2.32143700	1.10402900
H	1.85553100	3.41861900	-0.27355300
Ga	1.36021400	-0.40592400	0.01718300

GaCl₃-TS_{cis-c}

H	0.20885200	1.68563100	-0.97333200
C	0.30054900	1.32294600	-0.23206100
C	1.06218600	2.42687200	-0.16958600
C	-3.89500800	-0.92051000	0.32299800

C	-3.71712600	-0.26910500	-1.07503000
C	-0.98854500	1.47615400	1.01924900
C	-2.13483500	0.65458000	0.48476700
H	-0.73262700	1.12746200	2.02908100
H	-1.28891700	2.52956400	1.11376500
H	-2.45391300	-0.73730500	2.09167700
H	-3.88023100	-2.01585000	0.27718300
H	-4.85122600	-0.64139800	0.79160300
H	-3.20719500	-0.97468100	-1.73761900
H	-4.66881600	-0.00027800	-1.54319500
H	-3.36666300	1.90058400	-0.78629800
H	-2.07953200	1.08104000	-1.67014700
Cl	0.02245100	-1.61662800	-1.62794300
Cl	3.20344200	-0.15986700	-0.66786600
Cl	0.99396000	-1.50308600	1.97234600
C	-2.73905800	-0.36040700	1.11315400
C	0.81383400	3.88465900	0.05761400
C	-2.79774900	0.95866800	-0.84657600
H	1.99593600	2.18408700	-0.68552300
H	1.03607100	4.46262900	-0.84488100
H	-0.19111700	4.11655300	0.41245500
H	1.53281400	4.20759300	0.82453800
Ga	1.12205100	-0.58760900	-0.02039800

(GaCl₃)₂-TS_{trans-a}

H	-0.58900400	0.84211400	1.83975000
C	-1.49616000	1.61107100	1.63228400
C	-1.98362600	0.30703400	1.38696900
C	-0.98491800	3.92937000	-1.33766400
C	-0.13399900	4.64260500	-0.25199000
C	-1.08221700	2.61197000	0.62174000
C	-1.63908700	2.79867800	-0.58700000
H	-1.69558300	2.02629500	2.63083800
C	0.03396100	3.60644900	0.89001400
H	-2.46025600	2.21843600	-0.99893800
H	-0.36242200	3.52122600	-2.14748700
H	-1.71550200	4.59326700	-1.81433100
H	0.82705800	4.99367500	-0.63583600
H	-0.67838800	5.51680400	0.12133700
H	-0.03642100	4.06043800	1.88715900
H	1.01084700	3.10567900	0.84317200
Cl	0.50499400	-0.29614400	-1.50636100
Cl	-1.65331200	-3.10240700	0.11155400
Cl	-3.30021300	-0.27529400	-2.10764300
C	-2.64899500	-0.42789300	2.50324200
C	-4.17128800	-0.48759600	2.19146300
H	-2.49539700	0.07195900	3.46832900
H	-2.26723400	-1.45285900	2.56711900
H	-4.66802600	-1.02062100	3.00702200
H	-4.60618600	0.51362300	2.11613600
H	-4.38022800	-1.02772700	1.26273100
Cl	3.69360000	-2.28101500	-0.43254800
Cl	3.46959700	1.71211200	-0.30602500
Cl	1.35461900	-0.41543500	2.14856900
Ga	-1.71439400	-0.86140300	-0.50469600
Ga	2.52208500	-0.36968600	0.07878500

(GaCl₃)₂-TS_{cis-a}

H	0.93604500	-1.63090200	0.60732200
C	1.22603200	-0.49881000	1.43158000
C	2.05686800	-1.60132800	1.16364600
C	5.02247300	-0.92947900	-1.09276400
C	4.79529800	-2.44083100	-1.36980400
C	4.03292200	-0.62115300	-0.00133200
C	3.13625500	-1.61062600	0.15903300
H	2.03379100	-2.45391400	1.85114900
C	3.39218300	-2.76504100	-0.79142500
H	4.06209800	0.29709400	0.58183700
H	4.79150200	-0.30861400	-1.97050300
H	6.05398400	-0.69666900	-0.80509400
H	4.87304800	-2.68822200	-2.43149800
H	5.55428600	-3.02685500	-0.84047700
H	3.35323400	-3.74212900	-0.29316900
H	2.61906900	-2.78033800	-1.57236800
Cl	1.68793300	1.05010300	-2.21101200
Cl	-1.31946100	1.74042700	0.06128100
Cl	2.17342600	2.98210400	1.23024900
C	0.34647300	-0.46582000	2.64772600
C	0.29463400	-1.69175200	3.56336800
H	-0.66872900	-0.17022700	2.35442700

H	0.72837000	0.41118500	3.20065200
H	-0.37184400	-1.48355600	4.40498800
H	-0.10802600	-2.56655700	3.04062700
H	1.27846900	-1.94774400	3.97204700
Cl	-3.52275100	-0.74277500	1.83087500
Cl	-4.18037600	0.09539100	-2.03902600
Cl	-0.98840800	-1.91211900	-0.79435000
Ga	-2.72229600	-0.35227200	-0.31954900
Ga	1.16290200	1.24846000	0.04023500

(GaCl₃)₂-TS_{trans-b}

H	0.54413400	0.19450300	1.93374300
C	0.90080800	-0.84364200	2.71981500
C	1.61432800	-0.47207800	1.58067000
C	2.55513200	3.40525200	-0.57963500
C	4.05090600	3.47565900	-0.17302900
C	2.86080500	0.37300100	1.75619100
C	2.01461700	2.29105700	0.28466300
H	3.00188800	0.65947100	2.81146000
H	3.68787800	-0.32047100	1.53101600
H	0.94913900	2.10949800	0.38907700
H	2.42982700	3.15209600	-1.64244100
H	2.02869800	4.35424800	-0.42242600
H	4.70856000	3.70073400	-1.01729700
H	4.18890600	4.26937600	0.56964600
H	5.04126000	2.18677400	1.33402200
H	4.83884400	1.41059600	-0.23577700
Cl	0.52428700	-3.48877000	-0.38025800
Cl	-0.55161300	0.04729400	-1.54698200
Cl	3.19931100	-0.98718600	-1.77505700
C	2.99257000	1.57579900	0.85701200
C	-0.25436800	-1.78647400	2.81971800
C	4.36320400	2.10322300	0.47394000
H	1.24111100	-0.42445900	3.67451600
H	-0.62319600	-2.13968600	1.85584600
H	0.09804200	-2.65981700	3.38609500
H	-1.07241400	-1.33565400	3.38983300
Cl	-3.80617200	2.06641200	-1.35203300
Cl	-3.45234600	-1.50273100	0.48173800
Cl	-1.46187700	1.50077500	1.77873200
Ga	-2.59003000	0.56643800	-0.10216600
Ga	1.29762800	-1.29493700	-0.47942100

(GaCl₃)₂-TS_{cis-b}

H	0.84841000	-0.33926200	2.02769600
C	1.73402000	-1.19193600	2.50148100
C	2.03479400	-0.38354000	1.40403900
C	0.95858900	3.71356400	-0.22721400
C	2.34622100	3.82713100	-0.91252400
C	2.86437700	0.87057500	1.50952000
C	1.08894900	2.46092400	0.60354200
H	3.05987300	1.16794000	2.54902000
H	3.84103000	0.55447500	1.10695900
H	0.23677700	2.00866200	1.10468200
H	0.13098800	3.65964900	-0.94339800
H	0.74686500	4.57451200	0.42462200
H	3.88511900	3.57140900	0.65601200
H	4.03022100	2.41036200	-0.66288000
Cl	0.89914500	-3.34719100	-0.30182200
Cl	-0.58309700	-0.04479700	-1.55206900
Cl	3.19658600	-0.59292300	-2.11970700
C	2.35919400	2.04124900	0.69758300
C	2.12186100	-1.01190000	3.94094600
H	1.20273400	-2.12152300	2.28024500
C	3.30373700	2.96215800	-0.05392800
H	2.89272700	-1.75982900	4.16943700
H	2.52249200	-0.02321600	4.16963200
H	1.26679200	-1.22146000	4.59117800
Cl	-1.50432000	-0.14704500	2.12418900
Cl	-3.16578600	2.40066900	-0.27737100
Cl	-4.05658000	-1.49873500	-0.53942200
H	2.68627400	4.86192400	-1.01133400
H	2.28802400	3.40348300	-1.92068400
Ga	-2.58727000	0.18066500	0.02386400
Ga	1.48788400	-1.11058600	-0.63603600

(GaCl₃)₂-TS_{trans-c}

H	-0.10287400	1.68638900	0.51750900
C	-1.30763400	1.19776400	0.56196900
C	-0.78655600	1.79266000	1.70519800

C	-5.59439900	0.36952300	0.34101900
C	-5.90205000	1.15843100	-0.96031500
C	-2.18866700	2.00584400	-0.36752500
C	-3.60162100	1.46682900	-0.32507900
H	-2.17168000	3.07910800	-0.12156400
H	-1.80451600	1.91098400	-1.39123100
H	-3.73387700	0.57456500	1.64473700
H	-5.62143500	-0.71790700	0.18125200
H	-6.31121100	0.58153700	1.14343300
H	-6.48839600	0.57625900	-1.67638000
H	-6.48246500	2.05438800	-0.71432700
H	-4.52707300	2.58598300	-1.95765900
H	-4.17358200	0.89863000	-2.31949300
Cl	-1.82746700	-1.37096400	-2.13483400
Cl	1.26204300	-1.55049800	0.17035800
Cl	-2.06870000	-2.29601700	1.78064100
C	-4.19125200	0.80773600	0.68630600
C	0.00401800	1.13017400	2.78928500
H	-0.98795300	2.85979500	1.85574000
C	-4.52104300	1.57644600	-1.52650800
H	0.96457800	1.63303400	2.94605800
H	-0.57126500	1.23173300	3.71905400
H	0.17799000	0.06749800	2.60949400
Cl	3.77358900	0.66962800	1.93728900
Cl	4.45648800	-0.55435500	-1.83037700
Cl	1.60760300	2.03615100	-0.89377500
Ga	3.01910300	0.23186400	-0.21865300
Ga	-1.22505200	-0.96516000	0.06843200

(GaCl₃)₂-TS_{cis-c}

H	0.06141700	1.64054100	-0.14237900
C	-1.20944600	1.19150100	0.08691900
C	-0.50756900	2.01719600	0.96698900
C	-5.47118900	0.47580400	0.57507900
C	-5.91237000	0.80322300	-0.87757900
C	-2.16705000	1.72097200	-0.94917500
C	-3.56606900	1.25370900	-0.59988400
H	-2.13777700	2.81248600	-1.06172100
H	-1.89136400	1.29440600	-1.92270200
H	-3.49566500	1.05820100	1.55656500
H	-5.50081600	-0.60332100	0.78297500
H	-6.10903900	0.95315600	1.32857500
H	-6.55747900	0.03080200	-1.30488300
H	-6.47743400	1.74168900	-0.88352900
H	-4.65681300	1.80105300	-2.41108000
H	-4.32188500	0.07997800	-2.23750100
Cl	-1.98314600	-2.01606500	-1.70791500
Cl	1.30124500	-1.65285900	0.25133200
Cl	-1.88447800	-1.77735900	2.31438900
C	-4.04652000	0.97315800	0.62295500
C	-0.58848900	3.51060400	1.12930500
C	-4.59795600	0.98545500	-1.67865000
H	0.13539700	1.52626900	1.70122400
H	0.41904900	3.93668700	1.16500100
H	-1.16785400	4.00833400	0.35076700
H	-1.05863000	3.71166400	2.10027400
Cl	3.00828900	1.28747200	1.88588700
Cl	4.91774300	-0.83886200	-0.95472200
Cl	1.77550400	1.52342900	-1.67552400
Ga	-1.17463100	-1.02807100	0.23228000
Ga	3.00853200	0.16032500	-0.16301400

InBr₂-TS_{trans-a}

C	-3.44303400	1.05711300	0.19548400
C	-1.97314300	1.42866100	0.25795500
C	-1.44807300	1.18553200	1.48783800
C	-2.47543900	0.60063500	2.41903700
C	-3.62963500	0.18946900	1.46869800
C	-1.21342700	2.10676800	-0.80556800
C	0.06157100	1.65074200	-1.20145400
H	-1.61279900	3.04355200	-1.21433400
H	-1.09444200	1.32399200	-1.82177700
H	-0.46702900	1.52281000	1.82359400
H	-2.08285800	-0.22893500	3.01760400
H	-2.77923600	1.37784000	3.13574300
H	-3.52913700	-0.86776900	1.20410300
H	-4.61411400	0.32411000	1.92077700
H	-4.05024900	1.97360400	0.22585200
H	-3.71219000	0.52743000	-0.72486100
In	0.50297700	-0.29289600	-0.20823400
C	0.95776000	2.46815500	-2.08320300
C	2.06510500	3.10408800	-1.20168500

H	0.39757900	3.26062200	-2.59591200
H	1.42459500	1.83332100	-2.84370700
H	2.73060800	3.68366800	-1.84700400
H	1.64092700	3.78009300	-0.45310800
H	2.66817900	2.34838000	-0.68872100
Br	-0.76022500	-2.21622500	-1.19474700
Br	2.38948700	-0.42085400	1.41882200

InBr₂-TS_{cis-a}

C	-3.49084100	-0.33540700	0.35754100
C	-2.23544400	0.44559700	0.68928400
C	-1.57277100	-0.08155800	1.74993700
C	-2.26742000	-1.29833800	2.29979300
C	-3.62836500	-1.32943500	1.54581500
C	-1.80274500	1.67911100	0.01022100
C	-0.47614200	1.84960400	-0.43927600
H	-2.51578300	2.50864500	-0.04370100
H	-1.49478300	1.42016200	-1.21494700
H	-0.71120600	0.37576600	2.23836000
H	-1.66173800	-2.19659400	2.11289800
H	-2.38169000	-1.23226000	3.38727000
H	-3.88477400	-2.33404200	1.20405800
H	-4.42800600	-0.99981400	2.21458300
H	-4.36270400	0.32083900	0.24791100
H	-3.36575400	-0.85090500	-0.60509500
In	0.66350300	-0.04758000	-0.21893100
C	0.07106000	3.16593900	-0.91215700
C	-0.90730100	4.32876600	-1.10965900
H	0.67127000	2.99807200	-1.81565600
H	0.81459200	3.42246000	-0.13670500
H	-0.35552000	5.21131000	-1.44393100
H	-1.65676300	4.10387100	-1.87747300
H	-1.42284400	4.59767500	-0.18171100
Br	0.00257900	-1.83510200	-1.84267400
Br	2.62896000	-0.03802500	1.31389600

InBr₂-TS_{trans-b}

C	-3.24312400	0.93621400	0.41795900
C	-1.81959700	1.41946600	0.57132600
C	-1.25531800	0.91638000	1.70718700
C	-2.23187900	0.05935800	2.48338500
C	-3.35623800	-0.21287700	1.45156200
C	-1.14804100	2.36224500	-0.40729100
C	0.29547300	1.97324000	-0.64161200
H	-1.28418900	3.41399100	-0.11464200
H	-1.62817400	2.26358700	-1.39414100
H	-0.31264800	1.25800000	2.13893900
H	-1.78401600	-0.85129900	2.89318200
H	-2.59400200	0.64179000	3.34252500
H	-3.17615000	-1.16961300	0.94959100
H	-4.34461500	-0.26583500	1.91212600
H	-3.91761100	1.77276700	0.65849100
H	-3.48074500	0.62796200	-0.60641700
In	0.33850400	-0.20909700	-0.11388000
C	1.25283100	2.89916800	-1.06950500
C	2.65390500	2.56683100	-1.49430900
H	1.12393800	2.64546600	0.18292700
H	0.93379600	3.93713200	-1.22373100
H	2.96373200	1.56647100	-1.18065300
H	2.67755500	2.61044100	-2.59172700
H	3.36880500	3.30860600	-1.12710500
Br	-0.86298200	-1.59638100	-1.82113700
Br	2.23382600	-0.94744300	1.35338000

InBr₂-TS_{cis-b}

C	-3.17760100	-0.20760800	0.81783400
C	-1.95351600	0.67035200	0.93819100
C	-1.12881000	0.22501700	1.92929400
C	-1.70224800	-0.98731500	2.63055800
C	-2.82379400	-1.45527000	1.66686900
C	-1.72044500	1.90074100	0.08326700
C	-0.29361000	1.97142000	-0.40273300
H	-2.06644900	2.81036500	0.59417500
H	-2.32591900	1.83275800	-0.83607500
H	-0.28140600	0.78379300	2.33076300
H	-0.95807900	-1.76106800	2.84398200
H	-2.10212300	-0.66521000	3.60254500
H	-4.03760300	0.34140400	1.23177800
H	-3.42902200	-0.44521800	-0.22221600
In	0.45289600	-0.13830100	-0.18945600

C	0.32341900	3.15940300	-0.82316100
C	-0.30857500	4.51518600	-0.99499600
H	1.33231800	3.05527600	-1.23126900
H	0.52504600	2.80436800	0.36587200
H	-0.50965500	4.64747400	-2.06655900
H	-1.25034500	4.62978600	-0.45468400
H	0.38412500	5.30747000	-0.69760200
H	-3.68880800	-1.85873300	2.19672900
H	-2.44472400	-2.24494400	1.00976900
Br	2.67204900	-0.38117100	0.95030300
Br	-0.51856800	-1.65346700	-1.93471900

InBr₂-TS_{trans-c}

C	-3.15826200	1.01373800	0.45501500
C	-1.73998700	1.53487700	0.39430000
C	-1.08161400	1.30251200	1.56672700
C	-1.97270000	0.62403500	2.58218800
C	-3.17143900	0.13151800	1.72961200
C	-1.16348200	2.26335600	-0.80752200
C	0.27711900	1.83574300	-0.98457900
H	-1.28180000	3.35212900	-0.70939500
H	-1.72963600	1.96017100	-1.70019200
H	-0.11614900	1.73635600	1.83224100
H	-1.47209900	-0.17582200	3.13700800
H	-2.27591900	1.37407000	3.32664900
H	-3.02302500	-0.91627600	1.44726600
H	-4.11907100	0.19239900	2.26824300
H	-3.83706000	1.87590700	0.54353400
H	-3.45245400	0.47357800	-0.45168100
In	0.32826800	-0.24202000	-0.13790600
C	1.26153200	2.70589800	-1.48211900
C	2.74236700	2.41471400	-1.51808000
H	0.97709400	3.74989200	-1.65896800
H	0.70268700	2.04334100	-2.35091500
H	3.19464800	2.78912500	-2.44052900
H	3.20911700	2.95231000	-0.68365100
H	2.96506300	1.35051200	-1.40694200
Br	-1.04976200	-1.83111600	-1.50898400
Br	2.25582600	-0.85051400	1.33731200

InBr₂-TS_{cis-c}

C	2.83732700	-1.09880800	-0.88891300
C	1.85395300	-0.03572300	-1.32758900
C	0.87209400	-0.56739700	-2.10993800
C	1.08015100	-2.04902700	-2.33659600
C	2.14267500	-2.43089100	-1.27216400
C	1.97666900	1.42748800	-0.94406100
C	1.00953700	1.75950000	0.17385900
H	1.65776500	2.06817200	-1.78404400
H	3.01502400	1.70355600	-0.72481300
H	0.14959100	0.02110700	-2.67603000
H	0.16000200	-2.63744100	-2.26361800
H	1.45257100	-2.18596100	-3.36171600
H	1.65022400	-2.85085100	-0.38949700
H	2.85022600	-3.17759800	-1.63760800
H	3.77341800	-0.94377500	-1.44735400
H	3.09928600	-1.03697600	0.17451200
In	-0.45701400	0.05211700	0.16184900
C	1.13549400	2.89381900	0.98985800
C	2.11917000	4.02509900	0.84714000
H	1.61264300	1.82209900	1.43724100
H	0.32291600	3.06344900	1.70135300
H	2.45470000	4.37383400	1.82795600
H	2.98602200	3.77594200	0.23194900
H	1.58825700	4.86068400	0.37186600
Br	-2.68548200	0.52817400	-0.87466000
Br	-0.01570000	-1.52687000	2.06950600

InBr₃-TS_{trans-a}

H	-1.03781200	0.66172600	-2.14424700
C	-1.64580600	1.50330300	-1.46445700
C	-0.25839500	1.38140000	-1.20325200
C	-4.10181900	0.07605300	1.03664600
C	-4.99685200	0.17968300	-0.22672800
C	-2.75347300	0.87975800	-0.72587000
C	-2.81072700	0.71828600	0.60828700
H	-1.94618300	2.27050700	-2.19321500
C	-4.01348200	0.37777500	-1.40899800
H	-2.02795000	0.99585000	1.30846700
H	-3.90138900	-0.96941900	1.31521300

H	-4.54183100	0.55510900	1.91858800
H	-5.64017100	-0.69382900	-0.36078900
H	-5.64745800	1.05701800	-0.14126700
H	-4.39654200	1.07127000	-2.16901800
H	-3.80195900	-0.57077100	-1.92350800
C	0.66253400	2.34257100	-1.89840700
C	1.10288400	3.40698100	-0.86036300
H	0.17120500	2.84243200	-2.74514000
H	1.55415300	1.82156800	-2.26156400
H	1.78998900	4.10627800	-1.34541800
H	0.24644300	3.97156700	-0.47778900
H	1.62438100	2.95397000	-0.01224400
In	0.69180400	-0.23485300	0.08339500
Br	3.08961100	-0.34160000	-0.82815300
Br	0.60960100	0.60024300	2.51583000
Br	-0.65499700	-2.36608100	-0.43040700

InBr₃-TS_{cis-a}

H	-1.00675300	2.01817900	-0.73956700
C	-0.27538900	1.74183800	0.42579200
C	-1.66795900	1.97420300	0.31959100
C	-4.02562800	-0.96714000	0.65095900
C	-4.91507400	0.03286700	-0.13492700
C	-2.78314100	-0.17445800	0.95251700
C	-2.72825600	0.95912300	0.23100500
H	-2.02581700	3.00074400	0.46254800
C	-3.94157700	1.11564000	-0.66803800
H	-2.02753100	-0.50631100	1.65864400
H	-3.74812000	-1.83965700	0.04073600
H	-4.50881600	-1.35810100	1.55353400
H	-5.48252200	-0.44800500	-0.93594600
H	-5.63732900	0.49338300	0.54815700
H	-4.37134100	2.12551700	-0.63935000
H	-3.65208300	0.92266300	-1.71102500
C	0.64582800	2.87922700	0.77514900
C	0.09839600	4.30800000	0.85279300
H	1.52870300	2.82821400	0.12591500
H	1.03762500	2.57259800	1.76164700
H	0.90843200	4.99076600	1.12560000
H	-0.29884200	4.64463300	-0.11249200
H	-0.68960600	4.41549400	1.60633000
In	0.72583300	-0.24567700	-0.04740400
Br	0.62508900	-1.66915000	2.09155900
Br	3.12590700	0.44544500	-0.64795600
Br	-0.55199600	-1.14880100	-2.09648800

InBr₃-TS_{trans-b}

H	-0.47134300	-0.88857800	-2.43525600
C	0.08355000	-2.08226200	-2.00549500
C	0.40466400	-0.80450500	-1.53469000
C	4.13487900	-0.99017500	0.76255800
C	4.99346700	-0.05957200	-0.13383600
C	1.66808300	-0.15866200	-2.06587800
C	2.87828800	-1.18773300	-0.05099000
H	1.96524600	-0.57808400	-3.04182000
H	1.49149500	0.91288100	-2.22166200
H	2.12326900	-1.91723800	0.22860600
H	3.88597100	-0.51942500	1.72464100
H	4.64128500	-1.93350800	1.00083000
H	5.57276200	0.66662900	0.44327900
H	5.70493200	-0.66272400	-0.70909400
H	4.39682500	0.74644100	-2.11264500
H	3.68571600	1.61351400	-0.75308800
C	2.79327300	-0.31798700	-1.06835800
C	-1.03311300	-2.95777700	-1.53417500
H	0.73246400	-2.51307700	-2.77909200
C	3.98908100	0.61550100	-1.10139800
H	-1.47230200	-3.52239000	-2.36174300
H	-0.59508500	-3.68174400	-0.83204800
H	-1.81239900	-2.40717200	-1.00271300
In	-0.70634800	0.22538400	0.14879200
Br	0.40381300	2.50339800	0.47013400
Br	-3.07065500	0.35644300	-0.89894000
Br	-0.61061000	-1.39413600	2.14179400

InBr₃-TS_{cis-b}

H	-1.01827500	1.76401800	0.64986800
C	-0.67918700	1.36445600	-0.52084700
C	-0.40659700	2.68235500	-0.13374400
C	-5.16371400	0.31410500	0.45003400

C	-4.55553800	-1.11314700	0.38064800
C	-1.88060100	1.03669400	-1.39550200
C	-3.05368900	0.47871700	-0.61687400
H	-2.20330500	1.91013100	-1.97350700
H	-1.53033200	0.28355700	-2.11486800
H	-4.40881300	2.15388600	-0.68437100
H	-5.21633200	0.68910900	1.48359500
H	-6.18650100	0.35571400	0.05588900
H	-4.67044200	-1.66759900	1.31607100
H	-5.06450200	-1.68530600	-0.40256700
H	-2.71095800	-1.67609700	-0.71579200
H	-2.40654500	-0.97288800	0.86390800
C	-4.19251000	1.13706300	-0.36239900
C	-1.13469200	3.94275300	-0.49284300
H	0.49942000	2.82688400	0.46236100
C	-3.06813500	-0.91405700	-0.01213800
H	-1.22923200	4.59488800	0.38101200
H	-0.50948000	4.47675000	-1.22217500
H	-2.11696900	3.77299000	-0.93440200
In	0.88404200	-0.20763700	0.00526400
Br	3.01677100	1.23586000	0.05329900
Br	0.71093200	-1.92313200	-1.88276200
Br	0.27978800	-1.03345600	2.36657900

InBr₃-TS_{trans-c}

H	1.14262700	-1.80443500	-0.22518500
C	0.68694400	-1.01243100	-1.10302600
C	0.54515000	-2.38825200	-1.30455900
C	5.28851000	-0.67145900	-0.15153100
C	4.71123400	0.53088800	0.64403400
C	1.85336600	-0.32184400	-1.81609800
C	3.10100600	-0.25279200	-0.96378300
H	2.07842000	-0.84340100	-2.75600800
H	1.52385700	0.69377100	-2.07099900
H	4.39725600	-1.58293500	-2.05445400
H	5.41706600	-1.56237000	0.48211600
H	6.27485000	-0.45639600	-0.58064400
H	4.90302700	0.45785900	1.71814200
H	5.17966300	1.45642900	0.29272000
H	2.81431700	1.58555900	0.18272400
H	2.59289300	0.11900800	1.11709700
C	4.23702000	-0.92027100	-1.20650100
C	-0.53581500	-3.27467500	-0.76864500
C	3.19625400	0.56637200	0.31214200
H	1.28114800	-2.88053500	-1.95370600
H	-0.14512000	-4.26589800	-0.52066500
H	-1.04897900	-2.85002200	0.09678000
H	-1.27970800	-3.39563100	-1.56846000
In	-0.83517800	0.20495900	0.06734700
Br	-3.10206600	-0.42408400	-0.95720800
Br	-0.47950900	-0.75642400	2.44199400
Br	-0.21012700	2.65915900	-0.26512000

InBr₃-TS_{cis-c}

H	-0.30078100	2.21880300	-0.89326600
C	-0.23578300	1.76893200	0.31149600
C	0.51697700	2.89105300	-0.05789400
C	-4.34410500	-0.61514800	0.31433600
C	-4.20779800	0.08841900	-1.06385900
C	-1.53949800	1.88356600	1.07507700
C	-2.64853000	1.02609600	0.51762400
H	-1.28652500	1.53839900	2.08816800
H	-1.87459600	2.92645000	1.17116600
H	-2.92819700	-0.40573000	2.09826400
H	-4.27079600	-1.70603600	0.23304000
H	-5.31055300	-0.40348300	0.79625300
H	-3.70452600	-0.58417100	-1.76400500
H	-5.17525500	0.35648800	-1.49833000
H	-3.88935200	2.26213100	-0.75339200
H	-2.58414700	1.46852200	-1.63203900
C	-3.21723300	-0.02409300	1.12247100
C	0.25638100	4.34140100	0.21919300
C	-3.30802500	1.32842200	-0.81561000
H	1.46739000	2.67281800	-0.55670600
H	0.49135300	4.95214400	-0.65786100
H	-0.75765200	4.55436500	0.56041700
H	0.95633300	4.64060600	1.01203700
In	0.67827400	-0.29261500	0.00284400
Br	3.05831000	0.39482500	-0.75552900
Br	0.56384900	-1.31574800	2.35028400
Br	-0.52794300	-1.54436500	-1.88275800

(InBr₃)₂-TS_{trans-a}

H	-0.65026400	1.00906600	2.01746200
C	-1.50919600	1.86982500	1.93281400
C	-2.11204900	0.61360800	1.70549300
C	-1.17710400	4.28900200	-0.97657600
C	-0.11952200	4.86198200	0.00604600
C	-1.13041600	2.87788200	0.91898700
C	-1.82510500	3.17940100	-0.19139400
H	-1.55412700	2.25255100	2.96276900
C	0.09736300	3.75804400	1.07445300
H	-2.74515100	2.69624300	-0.50829100
H	-0.71545800	3.87350000	-1.88439000
H	-1.90074200	5.03997200	-1.31403700
H	0.81146500	5.13860800	-0.49474700
H	-0.51623500	5.76417800	0.48386500
H	0.19948300	4.16451700	2.08900900
H	1.01064000	3.17923100	0.88000800
Br	0.18341900	0.04993200	-1.55840900
Br	-2.12932100	-2.96846400	0.30560200
Br	-4.01682000	0.29015600	-1.77779100
C	-2.70402600	-0.11640400	2.86792100
C	-4.25139800	-0.04991700	2.74043900
H	-2.39928600	0.33184700	3.82238300
H	-2.39689000	-1.16803000	2.85686900
H	-4.69011000	-0.57865300	3.59128600
H	-4.61143500	0.98328800	2.75108200
H	-4.61021200	-0.53248100	1.82596800
Br	3.52191700	-2.48414000	-0.70925600
Br	3.71631200	1.89213200	-0.50282400
Br	1.44782500	-0.26112900	2.35335400
In	-2.13932800	-0.48884100	-0.24691700
In	2.50341800	-0.28669800	-0.02700000

(InBr₃)₂-TS_{cis-a}

H	-1.03748600	1.59660400	1.28060000
C	-1.52661800	0.28785500	1.68452100
C	-2.14877500	1.53929900	1.84483300
C	-5.20449100	2.18526700	-0.29701100
C	-4.70671900	3.63893900	-0.06917300
C	-4.27665700	1.36011600	0.55407700
C	-3.21214900	2.06933500	0.97059000
H	-1.98878900	2.08347800	2.78219400
C	-3.26223500	3.50481300	0.48223000
H	-4.46981500	0.31802900	0.80080600
H	-5.10199400	1.87322700	-1.34640000
H	-6.25766700	2.04549000	-0.02841100
H	-4.74843600	4.24242600	-0.97932500
H	-5.34022300	4.12849700	0.67817600
H	-3.04078100	4.23021700	1.27535400
H	-2.50655500	3.65706000	-0.30099900
Br	-2.25170000	0.21917700	-2.45012000
Br	0.80887300	-1.81883300	-0.50251900
Br	-3.17858500	-2.88040500	0.45766600
C	-0.68016900	-0.30334600	2.77205500
C	-0.41642400	0.51409200	4.03965700
H	0.26523600	-0.66037100	2.34474800
H	-1.22264600	-1.23375600	3.02041000
H	0.19832700	-0.07667800	4.72423100
H	0.13826700	1.43238000	3.81771800
H	-1.34171400	0.77758100	4.56350500
Br	3.47194800	-0.30571100	2.25649200
Br	4.24616400	0.18329300	-2.04293300
Br	1.06139100	2.28147100	0.01984400
In	2.65121100	0.21906100	-0.09894200
In	-1.76291600	-0.87124700	-0.21469700

(InBr₃)₂-TS_{trans-b}

H	0.71940000	0.53035300	2.08633000
C	1.22196700	-0.40449300	2.93336100
C	1.91853300	0.08216500	1.82656600
C	2.18095600	4.03081900	-0.38691300
C	3.58077400	4.44237300	0.14143100
C	2.95195400	1.16903400	2.05363900
C	1.83118100	2.83173300	0.46117100
H	2.95814000	1.49274000	3.10755300
H	3.91904900	0.66183700	1.90218000
H	0.82878600	2.41478100	0.48027000
H	2.21014400	3.74460200	-1.44823900
H	1.44246100	4.83680900	-0.30233700
H	4.24345300	4.79852500	-0.65221300

H	3.47132900	5.25701200	0.86585500
H	4.69216400	3.43054700	1.77121100
H	4.81989600	2.61221100	0.21510500
Br	1.67472400	-3.38229000	-0.03744000
Br	-0.25039400	0.05629400	-1.59107400
Br	3.97553800	-0.14837400	-1.54730800
C	2.88995500	2.36244300	1.13504300
C	0.27579600	-1.55748800	3.00177400
C	4.13482900	3.18481400	0.85725000
H	1.40820900	0.09812300	3.89013100
H	0.02222400	-1.98273100	2.02998000
H	0.77499400	-2.34153800	3.58860500
H	-0.63606300	-1.27721800	3.53745700
Br	-4.16558100	1.53645800	-1.57712500
Br	-3.11854100	-2.16237700	0.58587200
Br	-1.67041500	1.52599700	1.95454900
In	-2.59936300	0.22342400	-0.10791100
In	1.93862000	-0.85657100	-0.21399500

(InBr₃)₂-TS_{cis-b}

H	1.00712400	0.02267000	2.25494300
C	1.92984000	-0.71977100	2.84361200
C	2.25048900	0.09786000	1.75861500
C	0.91991600	3.99564600	-0.14242900
C	2.36591200	4.30421500	-0.61461800
C	2.91721500	1.44117100	1.90945700
C	1.09503900	2.77227800	0.72295500
H	2.95698500	1.78143600	2.95352100
H	3.96353700	1.23135000	1.63119100
H	0.24791400	2.20920700	1.10629800
H	0.22688600	3.82793400	-0.97461900
H	0.49396900	4.81691700	0.45314700
H	3.68284500	4.24871500	1.16252200
H	4.16792800	3.12187300	-0.10381800
Br	1.67946500	-3.23211400	0.05567200
Br	-0.22572000	0.08111500	-1.60197700
Br	3.98414100	0.02815800	-1.74186000
C	2.38254000	2.52969300	1.00885200
C	2.13465000	-0.46804600	4.30874900
H	1.53567700	-1.70982900	2.59796500
C	3.29503800	3.57065600	0.38610200
H	2.94877900	-1.12511600	4.64270000
H	2.40163500	0.56232200	4.54759200
H	1.23865900	-0.75556800	4.86779500
Br	-1.53398100	0.00765900	2.33753600
Br	-3.53526500	2.32811300	-0.59572700
Br	-3.79818100	-2.05656700	-0.66528300
H	2.57139200	5.37682800	-0.67170100
H	2.51779100	3.88813500	-1.61602600
In	-2.55691800	0.05312800	-0.06662300
In	2.03302000	-0.72888000	-0.31157800

(InBr₃)₂-TS_{trans-c}

H	0.38800000	-0.41833300	1.86597400
C	1.64360000	-0.22724500	1.52763900
C	1.09238000	0.51320900	2.56886500
C	6.00886700	-0.27428900	1.25068900
C	6.21538400	-1.81109700	1.33201600
C	2.41002600	-1.49334400	1.84152000
C	3.88421500	-1.27163800	1.58472300
H	2.24139500	-1.82744200	2.87703800
H	2.05212300	-2.29951200	1.18869800
H	4.11453500	0.87230300	1.79774600
H	6.21195300	0.11789600	0.24393300
H	6.66636200	0.27701100	1.93362400
H	6.89415100	-2.18511300	0.56081200
H	6.65060800	-2.06939400	2.30345500
H	4.65789400	-3.29291500	1.88044400
H	4.57085600	-2.76988900	0.20104400
Br	2.48261800	-1.47945500	-2.12227600
Br	-0.83618400	0.96658000	-1.34971300
Br	2.85132000	2.71241300	-0.83943200
C	4.54794500	-0.10367400	1.59373400
C	0.41151900	1.84271500	2.47874300
H	1.19139100	0.10466600	3.58129900
C	4.79721900	-2.42672100	1.22069300
H	-0.58333000	1.81203000	2.93650300
H	1.01274000	2.55523000	3.05892300
H	0.32973400	2.21952100	1.45750300
Br	-3.61121400	1.69124100	1.65433100
Br	-4.49418200	-1.20321000	-1.53948300

Br	-1.49777200	-1.90637700	1.51071800
In	-2.87887100	-0.19224200	0.10216100
In	1.78140600	0.41825700	-0.59754300

(InBr₃)₂-TS_{cis-c}

H	-0.20178900	1.74212000	-0.18230600
C	-1.51980900	1.43930800	0.02450600
C	-0.74514400	2.17183400	0.92635300
C	-5.85299000	1.31076200	0.43973700
C	-6.22142000	1.70685100	-1.01589000
C	-2.38319300	2.08289800	-1.02891500
C	-3.83851100	1.81323000	-0.70302000
H	-2.20364600	3.15964500	-1.14454200
H	-2.15046600	1.61913800	-1.99667100
H	-3.82938800	1.59567600	1.45255900
H	-6.04369700	0.24695500	0.64092000
H	-6.42389700	1.87297000	1.18830100
H	-6.96237600	1.03583700	-1.45862700
H	-6.64869200	2.71540800	-1.02203200
H	-4.81418200	2.53021500	-2.52089700
H	-4.73336300	0.77806900	-2.36634100
Br	-2.62589400	-1.79753400	-1.96253700
Br	0.86695200	-1.70461900	0.37520700
Br	-2.69570400	-1.48098200	2.42829500
C	-4.37201500	1.59512900	0.51051300
C	-0.65041800	3.66225100	1.09951200
C	-4.88291400	1.70692400	-1.79804700
H	-0.18078500	1.60413300	1.67016100
H	0.40056100	3.96299900	1.15337000
H	-1.15507700	4.23044700	0.31753100
H	-1.10688000	3.90997900	2.06631200
Br	2.90824200	1.44959900	2.09645600
Br	4.88837300	-1.11378400	-0.89461700
Br	1.63774600	1.65671600	-1.82920900
In	-1.74453600	-0.77127500	0.18242900
In	2.85804900	0.13316100	-0.10083800

InI₂-TS_{trans-a}

C	3.27713800	2.02489000	-0.64547300
C	1.80059300	2.08284500	-0.29789600
C	1.02378300	2.00099900	-1.40743500
C	1.85383600	1.85099500	-2.65347400
C	3.26284400	1.50332800	-2.10697700
C	1.25421500	2.34580000	1.04323600
C	0.19004000	1.58974600	1.58051300
H	1.62104700	3.22645600	1.58605600
H	1.50993900	1.35827000	1.81724100
H	-0.05051200	2.18218000	-1.43008400
H	1.45259900	1.09836500	-3.34157800
H	1.84060600	2.80436700	-3.20200900
H	3.39857300	0.41714300	-2.10525000
H	4.06513500	1.93448000	-2.70891600
H	3.70945500	3.03335100	-0.57061700
H	3.85263000	1.38233700	0.03024200
In	-0.29039000	-0.17410600	0.29314600
C	-0.51703100	2.02499700	2.83077900
C	-1.87142500	2.67018800	2.43684600
H	0.08258900	2.75332000	3.39247100
H	-0.70455300	1.16471000	3.48197600
H	-2.38543300	2.98069700	3.35045900
H	-1.72529100	3.55485200	1.80960400
H	-2.52262600	1.96895400	1.90632700
I	1.51155100	-2.15748700	0.48679200
I	-2.67304100	-0.29328700	-0.92190100

InI₂-TS_{cis-a}

C	-3.60633000	0.98331500	0.98361200
C	-2.18396700	1.45258500	0.75167900
C	-1.39382700	1.23283300	1.83013300
C	-2.14236700	0.56772100	2.95329300
C	-3.62848200	0.61308800	2.49423600
C	-1.71844300	2.13788500	-0.46595200
C	-0.51904200	1.78076000	-1.11923000
H	-2.27543000	3.02227500	-0.79317500
H	-1.76348100	1.33750500	-1.46084500
H	-0.36880900	1.58900900	1.93584300
H	-1.77651200	-0.46005100	3.09082300
H	-1.97275100	1.08029100	3.90644600

H	-4.14138600	-0.33438000	2.67103700
H	-4.16485500	1.38210200	3.05666300
H	-4.33825900	1.75875300	0.72632700
H	-3.83011400	0.12138400	0.33919100
In	0.39382800	-0.07499600	-0.27736300
C	0.09178400	2.61218900	-2.21087000
C	-0.71871800	3.78331300	-2.77750200
H	0.43687700	1.94810000	-3.01395400
H	1.02398300	2.98413100	-1.74909200
H	-0.13092700	4.28924300	-3.54804000
H	-1.64872800	3.44434000	-3.24867700
H	-0.96263900	4.52691500	-2.01167900
I	-0.91522800	-2.35808600	-0.80992800
I	2.83092200	0.20720000	0.79207000

InI₂-TS_{trans-b}

C	2.95546300	2.00224900	-0.66625400
C	1.58826000	2.13363100	-0.03469300
C	0.62409900	2.26504400	-0.98889500
C	1.21205800	2.26475900	-2.38311600
C	2.64664800	1.72175400	-2.15808200
C	1.36147400	2.15310800	1.46272900
C	0.11110800	1.38453200	1.84006500
H	1.38825500	3.17821500	1.86139200
H	2.18479600	1.61808400	1.96094100
H	-0.40824800	2.55873200	-0.79394400
H	0.63045500	1.67819600	-3.10130500
H	1.21751900	3.29829800	-2.75784300
H	2.66570900	0.64096700	-2.33484200
H	3.37771300	2.17577600	-2.82996600
H	3.49091300	2.95480800	-0.53066900
H	3.57178800	1.22881500	-0.19384300
In	-0.17512500	-0.06476300	0.13882500
C	-0.56643100	1.63454700	3.03726000
C	-1.70130300	0.82163100	3.58281000
H	-0.94050900	2.17924500	1.90853900
H	-0.18971400	2.43354200	3.68771000
H	-2.12739900	0.13911300	2.84302800
H	-1.29609800	0.22509200	4.41214200
H	-2.48673800	1.45802000	4.00089500
I	-2.65565400	-0.26309300	-0.89367300
I	1.67668400	-2.01768100	0.19394500

InI₂-TS_{cis-b}

C	-2.88975200	1.09893100	1.74062000
C	-1.62837900	1.64517000	1.11207800
C	-0.55636600	1.46079000	1.93264500
C	-0.95212700	0.79080100	3.22997000
C	-2.37217000	0.24651700	2.92695800
C	-1.60150800	2.35232700	-0.22794100
C	-0.39984800	1.94027600	-1.04424100
H	-1.70734100	3.43918100	-0.10216900
H	-2.47168100	2.04059700	-0.82873500
H	0.42017100	1.92669200	1.79291800
H	-0.24871400	0.01723600	3.55402100
H	-0.96340000	1.55171500	4.02332200
H	-3.50097600	1.94866500	2.08226300
H	-3.50894000	0.53403000	1.03426500
In	0.21865300	-0.04763500	-0.17625000
C	0.12412400	2.71649100	-2.08766900
C	-0.42980600	3.99280500	-2.65955300
H	0.94958200	2.26987900	-2.64848700
H	0.66136000	2.80601700	-0.93903100
H	-0.94907200	3.73108300	-3.59161600
H	-1.14265700	4.49436200	-2.00213900
H	0.37580300	4.68339900	-2.92467700
H	-3.03276300	0.29339400	3.79494800
H	-2.30980700	-0.80269900	2.61973400
I	-1.49546300	-1.99560800	-0.88969200
I	2.83413200	-0.34522400	0.38468100

InI₂-TS_{trans-c}

C	2.79679600	2.02053700	-0.90411400
C	1.45985500	2.18213500	-0.21537900
C	0.44656800	2.25131200	-1.12423800
C	0.96062400	2.17050300	-2.54324400
C	2.41764300	1.66881300	-2.36495500
C	1.30226500	2.31544000	1.28840000
C	0.06634400	1.54953500	1.71941000
H	1.27702600	3.37187600	1.59273000

H	2.18155600	1.86771300	1.77208900
H	-0.57807300	2.54037800	-0.88781600
H	0.35352000	1.53013500	-3.19112800
H	0.92220600	3.17854500	-2.98062700
H	2.45577300	0.58241000	-2.49869400
H	3.10304600	2.11000300	-3.09131800
H	3.33713900	2.97723500	-0.83718800
H	3.43408100	1.26690600	-0.42759900
In	-0.15783900	-0.07960900	0.17988000
C	-0.72153300	1.96921200	2.80184200
C	-2.04006500	1.36594900	3.21185100
H	-0.45585300	2.91274600	3.29317900
H	0.18699000	1.15678500	3.06017500
H	-2.11909400	1.29327200	4.30027500
H	-2.83481900	2.04212000	2.87254900
H	-2.21222500	0.38386000	2.76451900
I	1.81946600	-1.90222000	0.36629100
I	-2.60150700	-0.51804000	-0.85256800

InI₂-TS_{cis-c}

C	-2.74810200	1.32211500	1.56508000
C	-1.32687800	1.77832700	1.31352300
C	-0.46797900	1.23728000	2.22033600
C	-1.18737500	0.37274700	3.23065800
C	-2.60139000	0.19052100	2.61596700
C	-0.94651600	2.73976100	0.20420200
C	-0.38275500	1.97921500	-0.97963900
H	-0.12247900	3.39373800	0.53471000
H	-1.78009100	3.40318600	-0.05585400
H	0.57195500	1.54000500	2.33952000
H	-0.67889000	-0.57509100	3.43550600
H	-1.21681000	0.91694000	4.18518500
H	-2.67005700	-0.78223200	2.12004500
H	-3.38924900	0.22479900	3.37102800
H	-3.31835500	2.17941500	1.95391400
H	-3.26637700	0.99771400	0.65363500
In	0.21144300	-0.03252200	-0.14661500
C	-0.29734000	2.52332100	-2.26894100
C	-0.61870900	3.92816000	-2.70008800
H	-1.29476300	1.78658100	-1.98797400
H	0.19743200	1.90196200	-3.02021500
H	-1.11002000	3.93347100	-3.67738100
H	-1.22687000	4.47862000	-1.97987200
H	0.33710700	4.45652200	-2.81823000
I	-1.48460900	-2.00205700	-0.87006900
I	2.84440200	-0.31286300	0.32145600

InI₃-TS_{trans-a}

H	1.18741300	-0.74704400	2.31940500
C	1.78919300	0.34021400	2.33764300
C	0.41371800	0.39189400	1.99556100
C	4.42267200	0.77343300	-0.34919800
C	5.25939400	0.12643100	0.78623900
C	2.95474500	0.31721200	1.44305700
C	3.07446400	0.98633800	0.28248400
H	2.03344100	0.49117900	3.39957600
C	4.22052000	-0.45166900	1.78158200
H	2.30398600	1.60508400	-0.16751800
H	4.30791000	0.10079300	-1.21231600
H	4.86036800	1.70164200	-0.73380200
H	5.95306900	-0.63408600	0.41837900
H	5.85420600	0.89888600	1.28594200
H	4.52622300	-0.33432400	2.82948300
H	4.05725100	-1.52693400	1.61904500
C	-0.54352700	0.70000700	3.11400900
C	-0.98236900	2.17997100	2.97782700
H	-0.07912200	0.55031200	4.09905800
H	-1.43208700	0.06454900	3.04486100
H	-1.67910000	2.41520900	3.78768500
H	-0.12677900	2.85956000	3.04849400
H	-1.49214000	2.36564800	2.02826600
In	-0.48200100	-0.07255700	-0.05929700
I	-3.07050300	-0.85258700	0.51831900
I	-0.39993800	2.29731400	-1.49530400
I	1.01177200	-2.16997500	-1.08105700

InI₃-TS_{cis-a}

H	1.14385400	-0.84163300	2.25406600
C	0.42814200	0.32552600	1.96403800
C	1.80487100	0.22122100	2.28176200

C	4.38564100	0.65143000	-0.45251900
C	5.21824600	-0.09528200	0.62389100
C	3.06474300	0.89158300	0.22485000
C	2.94286200	0.17125700	1.35390500
H	2.08907900	0.33691700	3.33439800
C	4.17938400	-0.66862000	1.62267100
H	2.31262500	1.56818900	-0.16991300
H	4.21773900	0.03428000	-1.34758100
H	4.85794500	1.57843900	-0.79693800
H	5.85855700	-0.87165800	0.19720100
H	5.86846700	0.61829700	1.14164400
H	4.51767200	-0.61177300	2.66566600
H	3.96203000	-1.72718800	1.41917600
C	-0.55242200	0.63982300	3.06446700
C	-0.07734900	0.69463900	4.52043200
H	-1.42101900	-0.02222700	2.96170400
H	-0.94422300	1.62693500	2.76160700
H	-0.92564000	0.94006000	5.16621000
H	0.31827300	-0.27108900	4.85774900
H	0.69091600	1.45849100	4.68353600
In	-0.50033600	-0.01883100	-0.09961500
I	-0.44464900	2.50354800	-1.25328200
I	-3.07050500	-0.87454800	0.46063200
I	0.94167200	-2.00414800	-1.38599900

InI₃-TS_{trans-b}

H	-0.34737100	0.25546500	2.70743800
C	0.25669300	1.50089400	2.66941300
C	0.57258000	0.40406900	1.85964300
C	4.50628400	1.26495900	0.09386700
C	5.30845300	0.12791400	0.78031900
C	1.79589300	-0.40180100	2.25177500
C	3.15813700	1.19126900	0.77064800
H	1.99827500	-0.33342400	3.33406000
H	1.62477100	-1.46293200	2.03139000
H	2.40019300	1.95616100	0.62643600
H	4.39428200	1.09402500	-0.98658000
H	4.98518800	2.24568800	0.20365000
H	5.98457200	-0.38719100	0.09216700
H	5.92019700	0.54900300	1.58603800
H	4.54129600	-1.23033300	2.35713200
H	4.03246600	-1.67803800	0.73137200
C	3.00796800	0.06175300	1.47734800
C	-0.81223600	2.51998100	2.43763900
H	0.87643000	1.66251300	3.56110300
C	4.24068900	-0.81819400	1.38457500
H	-1.28253300	2.82321100	3.37771000
H	-0.31902400	3.40584700	2.01211800
H	-1.57457200	2.19150000	1.72854100
In	-0.48987700	-0.10030400	-0.09586100
I	0.70825700	-2.35948500	-1.10485700
I	-3.06131200	-0.58353600	0.87423900
I	-0.31556700	2.16412100	-1.67535900

InI₃-TS_{cis-b}

H	-1.56701900	-1.51360900	-0.81706400
C	-1.13536300	-1.17754400	0.38520800
C	-1.14807900	-2.50188600	-0.07123600
C	-5.93648600	-0.66593400	0.21032700
C	-5.36510500	0.45475300	-0.69922700
C	-2.25075000	-0.65632700	1.28717400
C	-3.60710500	-0.51568600	0.62856300
H	-2.32910800	-1.31835900	2.15964400
H	-1.94135300	0.32737200	1.66221500
H	-4.85018600	-1.65657700	1.96672700
H	-6.27660000	-1.53694200	-0.37044000
H	-6.80221900	-0.33031400	0.79391400
H	-5.75346500	0.41297100	-1.72072000
H	-5.63970400	1.43130200	-0.28668300
H	-3.29623100	1.25660100	-0.61777000
H	-3.44267500	-0.23893700	-1.52485800
C	-4.75743600	-1.03355200	1.07975200
C	-2.11157900	-3.59730900	0.28824200
H	-0.29340100	-2.80379400	-0.68556800
C	-3.82380600	0.29585500	-0.63866100
H	-2.29513000	-4.25221600	-0.56872400
H	-1.62731600	-4.20762800	1.06330500
H	-3.05800200	-3.22039200	0.67650400
In	0.69996400	0.11089300	-0.01579100
I	1.94607500	-0.12523600	2.43738200
I	-0.18552500	2.64786800	-0.62527900

I	1.93168500	-1.22824400	-2.10979400
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InI₃-TS_{trans-c}

H	1.72920100	-1.13796100	0.92926900
C	1.46883000	-0.60780600	-0.19121300
C	1.84814400	-1.95369000	-0.16942800
C	6.22193400	-0.58661500	-0.73840300
C	6.13432500	-0.02267000	0.70608100
C	2.52444300	0.43272300	-0.57239400
C	3.97137500	0.07262500	-0.35986500
H	2.33166100	0.62793800	-1.63787500
H	2.28356200	1.37320100	-0.06211600
H	4.61682100	-0.39700700	-2.35903500
H	6.42990100	-1.66734600	-0.74840700
H	7.02242200	-0.11746200	-1.32306200
H	6.66882500	-0.63865500	1.43485000
H	6.58440200	0.97522200	0.73325500
H	4.37285400	1.00280300	1.57872800
H	4.26951200	-0.74902300	1.63764300
C	4.85016700	-0.30108600	-1.30087600
C	0.95474800	-3.13487400	0.03486900
C	4.61880900	0.09245900	1.01750100
H	2.90254700	-2.17675500	-0.37383500
H	1.46642300	-3.93087100	0.58349600
H	0.01398600	-2.88625300	0.53089900
H	0.71073700	-3.51938900	-0.96618000
In	-0.69653800	0.09640800	-0.00576200
I	-1.93496300	-1.15451400	-2.14144700
I	-1.46306100	-0.84492900	2.49658300
I	-0.61762000	2.84040800	-0.17085100

InI₃-TS_{cis-c}

H	0.56945300	-1.55740100	1.97092400
C	0.43415200	-0.28040000	1.95266100
C	-0.28245900	-1.04146900	2.88465800
C	4.72371100	0.32738000	-0.02054500
C	4.55115200	-1.17941100	0.31202100
C	1.70070200	0.46330600	2.33198900
C	2.88665300	0.12873700	1.46055600
H	1.44596300	1.52487000	2.20794100
H	1.96050800	0.32297400	3.39101600
H	3.24434500	2.00329600	0.46908600
H	4.76299900	0.51461200	-1.10002800
H	5.65285200	0.74088600	0.40023600
H	4.10291600	-1.68883500	-0.54610300
H	5.49986200	-1.67639400	0.53453600
H	4.07406700	-1.37339100	2.46840100
H	2.85554900	-2.07071500	1.40564500
C	3.52559400	0.96669600	0.63513200
C	-0.01977300	-1.25120300	4.34617300
C	3.56032000	-1.23132300	1.50412000
H	-1.20649500	-1.49590100	2.51163700
H	-0.19951500	-2.29391200	4.62542800
H	0.97713400	-0.94742900	4.66780500
H	-0.75771300	-0.64445700	4.88963700
In	-0.48123500	0.06587100	-0.12276100
I	-3.05230500	-0.94399700	0.25549200
I	-0.37130100	2.81123000	-0.38182100
I	0.85980000	-1.41439900	-2.03068000

(InI₃)₂-TS_{trans-a}

H	-0.74374600	1.04778800	2.15375900
C	-1.54585000	1.98795000	2.15846200
C	-2.19708200	0.76419800	1.89545100
C	-1.17604800	4.58378000	-0.58496600
C	-0.10733900	5.06883900	0.43199100
C	-1.14526300	3.03934300	1.20452600
C	-1.83761400	3.42976300	0.12025600
H	-1.51894000	2.30465100	3.21119800
C	0.09733800	3.88710800	1.41565900
H	-2.76719900	2.98556300	-0.22356200
H	-0.72357200	4.22923100	-1.52279900
H	-1.89044600	5.36693100	-0.86409300
C	0.82535100	5.36936400	-0.05166000
H	-0.49017100	5.93878600	0.97629700
H	0.21155000	4.21680000	2.45638300
H	0.99993900	3.30905400	1.17407400
I	0.01172400	0.26708000	-1.66364700
I	-2.47285300	-2.96569300	0.38012500
I	-4.49527600	0.71677700	-1.54341500

C	-2.76296000	0.01500900	3.06546200
C	-4.30789100	0.15467000	3.04044200
H	-2.38002100	0.41060900	4.01544600
H	-2.50408100	-1.04736200	3.00226900
H	-4.71897400	-0.37888800	3.90218400
H	-4.61734300	1.20263000	3.10224000
H	-4.74572500	-0.28123700	2.13719500
I	3.57142400	-2.55040500	-0.99196600
I	3.89101000	2.11474800	-0.48030400
I	1.52475700	-0.37011700	2.55584800
In	-2.38353000	-0.27470000	-0.09875200
In	2.53308000	-0.22559700	-0.05542300

(InI3)2-TScis-a

H	-1.20076200	1.30344600	1.84882000
C	-1.73638000	-0.04135000	1.85324700
C	-2.28824000	1.11531600	2.43707900
C	-5.42658600	2.54859400	0.87659200
C	-4.83536400	3.82018100	1.54534400
C	-4.48914600	1.45376300	1.30945900
C	-3.36577700	1.94164100	1.86436100
H	-2.04750800	1.32644800	3.48503800
C	-3.37248400	3.45788600	1.91891000
H	-4.71826800	0.39726000	1.19083800
H	-5.42050100	2.61703000	-0.22094300
H	-6.46372300	2.35232200	1.17156800
H	-4.89070400	4.69724600	0.89568500
H	-5.39996600	4.05161700	2.45474400
H	-3.07843200	3.84612700	2.90256500
H	-2.65050800	3.86313200	1.19631400
I	-2.63036400	1.31491500	-2.18732500
I	0.52073700	-1.67043800	-1.07446700
I	-3.79600000	-2.73986500	-0.14944500
C	-0.86624000	-0.95921600	2.66370200
C	-0.52450600	-0.58964000	4.11008800
H	0.04993900	-1.17967000	2.10158700
H	-1.42357500	-1.91247300	2.63618500
H	0.09256000	-1.38130100	4.54396800
H	0.05512500	0.33849600	4.16415200
H	-1.41892300	-0.48436000	4.73390600
I	3.61233800	-1.31574500	2.13273800
I	4.31792800	0.65079700	-2.09322600
I	1.21709200	2.35542700	0.92221400
In	2.67271700	0.14017100	0.00169700
In	-2.09859800	-0.58625600	-0.30277900

(InI3)2-TStrans-b

H	0.87451600	0.77381600	2.15051300
C	1.39687800	-0.14125600	3.02974800
C	2.08999000	0.39113300	1.94041200
C	2.03856800	4.48463200	-0.02849700
C	3.32273200	5.02931800	0.65157300
C	3.05008500	1.53509600	2.21527900
C	1.81192300	3.16583200	0.67132400
H	3.05547200	1.79253500	3.28778900
H	4.05136400	1.12069500	2.01439400
H	0.88468300	2.61165300	0.56092500
H	2.18087100	4.32284900	-1.10677500
H	1.18524100	5.16570600	0.07282700
C	3.97965900	5.55598000	-0.04632000
H	3.04464700	5.73993700	1.43774100
H	4.45942000	4.01768400	2.26387100
H	4.80624200	3.39016400	0.65423500
I	2.37268000	-3.30968800	0.17977500
I	-0.09480500	0.09719000	-1.68121100
I	4.41111900	0.42754500	-1.45911100
C	2.87515600	2.78314200	1.38999000
C	0.50503100	-1.33591600	3.06945600
C	4.00388100	3.79294500	1.29003900
H	1.53686400	0.36075100	3.99498600
H	0.25738500	-1.73833300	2.08671700
H	1.04829500	-2.11677300	3.62092200
H	-0.41173900	-1.11729400	3.62492500
I	-4.42475100	1.24753900	-1.77088500
I	-3.00427800	-2.50317000	0.71672800
I	-1.88091400	1.69919400	2.09558400
In	-2.64857800	0.09352100	-0.07238900
In	2.26881900	-0.58362700	-0.09657700

(InI3)2-TScis-b

H	1.13315100	0.37764200	2.33509700
C	1.96570100	-0.43388300	2.99718700
C	2.39007900	0.35219000	1.92378300
C	1.32927100	4.39691100	0.14867600
C	2.81161300	4.73238800	-0.16705300
C	3.14129000	1.64642300	2.11845200
C	1.42458700	3.09480600	0.90526200
H	3.20305700	1.94531000	3.17456000
H	4.17357800	1.38658100	1.83166800
H	0.54415000	2.51029900	1.15966200
H	0.71170100	4.31719300	-0.75345800
H	0.85692300	5.16427500	0.78019300
H	3.97835200	4.48408600	1.69637800
H	4.55612900	3.47777000	0.37015000
I	1.94757200	-3.22214400	0.25978700
I	-0.03256400	0.37846400	-1.66313900
I	4.49915900	0.26497800	-1.55363800
C	2.68111100	2.80835500	1.27218300
C	2.11147500	-0.19230100	4.46943500
H	1.50957400	-1.39323600	2.73821600
C	3.64906000	3.89011300	0.82928500
H	2.85751800	-0.90791700	4.84125100
H	2.44023000	0.81570100	4.72480300
H	1.16986500	-0.41545100	4.98113600
I	-1.68106600	0.47122900	2.54738200
I	-4.06614900	2.14709200	-1.00450000
I	-3.44755300	-2.49861500	-0.51091000
H	3.02606300	5.80259000	-0.09790900
H	3.04549900	4.41739500	-1.18919700
In	-2.59338100	0.04675500	-0.07978700
In	2.29013600	-0.52482500	-0.15592400

(InI3)2-TStrans-c

H	0.59093000	-0.15898800	1.98734600
C	1.85599000	-0.05143900	1.69640200
C	1.29403400	0.87733100	2.56877800
C	6.23317700	-0.12281100	2.09128200
C	6.39115000	-1.62288100	2.45985800
C	2.56294100	-1.25432000	2.28743000
C	4.06158700	-1.06137600	2.23245700
H	2.24038800	-1.44200500	3.32385500
H	2.29757900	-2.15023200	1.71252800
H	4.30060000	1.08704700	2.11089100
H	6.60314500	0.09536000	1.07928400
H	6.78503400	0.53881600	2.76996400
H	7.17695500	-2.11734200	1.88231900
H	6.65923600	-1.71206300	3.51823400
H	4.73268000	-2.99767900	2.99039400
H	4.92989700	-2.77156000	1.25581400
I	3.01265900	-2.06319500	-1.69942100
I	-0.58644400	0.65731100	-1.65138100
I	3.38995800	2.58561000	-1.08348400
C	4.74040800	0.09413200	2.15729300
C	0.64903500	2.18054000	2.22542300
H	1.33795600	0.64790500	3.64011700
C	4.99608500	-2.25622100	2.22479200
H	-0.35161000	2.25484600	2.66596500
H	1.25943200	2.97381500	2.67791400
H	0.59047900	2.36793900	1.15188500
I	-3.58598400	2.27714200	1.29521800
I	-4.63108100	-1.42268400	-1.43336000
I	-1.55720400	-1.71593500	2.04358300
In	-2.85592300	-0.10537600	0.13860900
In	2.11959600	0.22413500	-0.51412000

(InI3)2-TScis-c

H	-0.40521800	1.71738900	0.58045000
C	-1.71761500	1.44684500	0.58515300
C	-1.01074900	1.69271500	1.76434900
C	-6.05124000	1.86132000	1.08437500
C	-6.29788300	2.90965100	-0.03330200
C	-2.46710400	2.53568000	-0.14112500
C	-3.94964000	2.41848800	0.14442800
H	-2.10712100	3.54325900	0.10834300
H	-2.30848100	2.41196200	-1.22028000
H	-4.03906100	1.29509500	1.99412900
H	-6.44652100	0.87096200	0.81575600
H	-6.52594700	2.13638800	2.03389000
H	-7.14886300	2.65407200	-0.67054500
H	-6.51078700	3.88319900	0.42162900
H	-4.72067400	4.01308800	-1.13617000
H	-4.99242500	2.38184300	-1.74103200

I	-3.37430000	-0.75923200	-2.50787000
I	0.64032700	-1.73706500	-0.77849700
I	-2.88895500	-2.16223400	1.99229100
C	-4.54529800	1.80815500	1.18056700
C	-0.88891600	2.96955700	2.54371100
C	-4.96786200	2.98962600	-0.82494800
H	-0.51958900	0.83612700	2.23360400
H	0.16492500	3.18625900	2.74693300
H	-1.35740100	3.82790300	2.06160100
H	-1.37424400	2.80167800	3.51397900
I	2.72983200	0.20467300	2.73493400
I	5.02711100	-0.69029400	-1.29282400
I	1.69150400	2.58333300	-0.93948800
In	-2.04132300	-0.65505800	-0.13102500
In	2.79472700	0.17285300	-0.02437200

GaBr₃-TS_{trans-a}

H	-0.94066100	0.63045800	-2.05313200
C	-1.54453200	1.43645000	-1.32972500
C	-0.15422100	1.30239700	-1.07451100
C	-4.07911600	-0.09554400	1.02802600
C	-4.95827400	0.17395800	-0.22184000
C	-2.67629900	0.79790200	-0.64602300
C	-2.75218600	0.51163300	0.66605200
H	-1.82828700	2.24331600	-2.01997400
C	-3.95692700	0.43184400	-1.37707100
H	-1.95921500	0.67650200	1.38869200
H	-3.93714100	-1.17167200	1.20956500
H	-4.49907600	0.32196000	1.95026800
H	-5.64557800	-0.64762400	-0.44013400
H	-5.56318400	1.07192100	-0.05454000
H	-4.29744700	1.21556000	-2.06652400
H	-3.79484600	-0.47186500	-1.98238100
C	0.75004100	2.31017400	-1.72816400
C	1.18146100	3.33975500	-0.65197900
H	0.24169300	2.83545300	-2.54840000
H	1.64559300	1.82011100	-2.12095700
H	1.84913400	4.07107400	-1.11687700
H	0.31847500	3.87153900	-0.23837700
H	1.71829200	2.86068800	0.17081600
Ga	0.74403500	-0.21850300	0.04130800
Br	3.00853100	-0.37604400	-0.77920400
Br	0.69442100	0.52262000	2.35141600
Br	-0.48102500	-2.25529700	-0.41070400

GaBr₃-TS_{cis-a}

H	-0.89836900	1.68738000	-1.25248400
C	-0.15613500	1.63754300	-0.05711800
C	-1.54914500	1.86236000	-0.20130400
C	-4.00141100	-0.87439900	0.70240700
C	-4.88650000	0.03101700	-0.19485100
C	-2.71079600	-0.11190400	0.81527900
C	-2.64532500	0.89334200	-0.07572100
H	-1.87653300	2.90580300	-0.26495900
C	-3.89715400	0.97034800	-0.93256900
H	-1.93346700	-0.36635400	1.52892900
H	-3.79486400	-1.84820800	0.23359700
H	-4.45291400	-1.08889200	1.67781400
H	-5.51136400	-0.54143200	-0.88544600
H	-5.55603200	0.62644900	0.43550100
H	-4.28329700	1.99264900	-1.03977600
H	-3.67536300	0.60933100	-1.94750000
C	0.76949600	2.82125300	0.05691600
C	0.21318300	4.24010600	-0.09280000
H	1.62651500	2.66066300	-0.60796100
H	1.19916400	2.69112300	1.06557400
H	1.02636100	4.95998000	0.03892600
H	-0.21244900	4.41136500	-1.08899800
H	-0.55369400	4.47088500	0.65487900
Ga	0.77540100	-0.22934000	-0.01700100
Br	0.76918000	-0.77415100	2.35053900
Br	3.01618400	0.11915700	-0.84411200
Br	-0.41274700	-1.77012600	-1.45335500

GaBr₃-TS_{trans-b}

H	-0.51036300	-0.86332500	-2.27951800
C	0.09999300	-2.04823500	-1.80097900
C	0.34122200	-0.73421700	-1.38108300
C	4.14641300	-0.88941900	0.82261600
C	4.98987800	-0.00522400	-0.13293700

C	1.58720300	-0.05647400	-1.92106400
C	2.85098900	-1.07226100	0.06842900
H	1.86050800	-0.45103600	-2.91389100
H	1.39137000	1.01476100	-2.05026900
H	2.08593900	-1.76722500	0.40297500
H	3.95134100	-0.38758300	1.78149300
H	4.63861400	-1.83947100	1.06440900
H	5.61455500	0.71734600	0.39986900
H	5.65816500	-0.64182400	-0.72381500
H	4.32911400	0.77321600	-2.10231300
H	3.70044700	1.68791900	-0.73431300
C	2.74495100	-0.22566500	-0.96552100
C	-0.97461500	-2.96525300	-1.32286500
H	0.78037100	-2.46244800	-2.55505000
C	3.96197600	0.67441000	-1.07194600
H	-1.34850400	-3.59709700	-2.13361900
H	-0.51156600	-3.62282700	-0.57198900
H	-1.79969200	-2.44155700	-0.83668300
Ga	-0.77130300	0.21061800	0.10786000
Br	0.14921900	2.39863200	0.45178600
Br	-2.99303800	0.28676700	-0.90604900
Br	-0.71098100	-1.22008500	2.05829600

GaBr₃-TS_{cis-b}

H	-1.11332900	-1.00621500	-1.07826500
C	-0.71216700	-0.91954900	0.15338900
C	-0.82831800	-2.16313500	-0.47847900
C	-5.49806500	-0.11696800	0.13577200
C	-4.87750800	1.00371100	-0.74166600
C	-1.79159300	-0.39523000	1.09723100
C	-3.15210200	-0.14478700	0.48510100
H	-1.87888300	-1.10471700	1.93053800
H	-1.42444700	0.54725200	1.52130000
H	-4.43095600	-1.26550500	1.80547800
H	-5.91820000	-0.93339500	-0.47132500
H	-6.31911300	0.25024700	0.76335000
H	-5.29474900	1.03178200	-1.75224000
H	-5.07706200	1.97707300	-0.28125700
H	-2.75776800	1.66537100	-0.67941900
H	-3.02725000	0.23111100	-1.65595900
C	-4.32200700	-0.60608400	0.94710400
C	-1.90883300	-3.18877100	-0.31826200
H	0.02023900	-2.45040300	-1.10731100
C	-3.34847900	0.74325900	-0.73320600
H	-2.12556300	-3.68287200	-1.27016500
H	-1.51037700	-3.95826700	0.35870400
H	-2.82392800	-2.78150000	0.11191000
Ga	1.07966300	0.12165700	0.00609400
Br	2.06751800	-0.34751600	2.15644600
Br	0.51404400	2.43977900	-0.33338300
Br	2.24261600	-0.87986300	-1.87066800

GaBr₃-TS_{trans-c}

H	1.17397500	-0.91455000	0.98572600
C	0.93144600	-0.44163900	-0.14592800
C	1.33670400	-1.78021900	-0.10798600
C	5.68301800	-0.31662100	-0.64753600
C	5.56717400	0.26849800	0.78661300
C	1.96252200	0.62067800	-0.53798100
C	3.41380800	0.29685200	-0.30321100
H	1.77651500	0.79692200	-1.60729300
H	1.68892500	1.55843800	-0.04108600
H	4.09121400	-0.19069400	-2.28724000
H	5.91613400	-1.39222400	-0.63766600
H	6.47868100	0.16150700	-1.23154800
H	6.10731600	-0.32344400	1.53099700
H	5.99462700	1.27653700	0.80211800
H	3.77361200	1.26914400	1.62248600
H	3.70890800	-0.48295200	1.71193500
C	4.31115300	-0.07208600	-1.22849200
C	0.46922300	-2.97404500	0.10815600
C	4.04604900	0.35492100	1.08020600
H	2.40053800	-1.97623000	-0.28580800
H	0.99711600	-3.75514400	0.66257200
H	-0.47894700	-2.73632700	0.59422500
H	0.23653800	-3.36873300	-0.89230900
Ga	-1.06745100	0.13669100	-0.00924500
Br	-2.15772300	-1.02450900	-1.83043100
Br	-1.75730600	-0.64288600	2.19442300
Br	-1.14499300	2.52745900	-0.21152200

GaBr₃-TS_{cis-c}

H	-0.35072900	2.04730300	-0.66856000
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C	-0.19184200	1.55539200	0.48140200
C	0.47100900	2.75639200	0.19909900
C	-4.32972200	-0.79411900	0.22112100
C	-4.20911400	0.11754000	-1.03047600
C	-1.46921000	1.51335900	1.30353400
C	-2.60429900	0.77196500	0.64101000
H	-1.18596400	0.99259100	2.22749700
H	-1.79681200	2.52130000	1.59462600
H	-2.85769400	-0.89775900	1.97032500
H	-4.28072900	-1.85930900	-0.03399400
H	-5.28150200	-0.64519400	0.75339900
H	-3.71550400	-0.43707400	-1.83374100
H	-5.18045300	0.45229800	-1.40632400
H	-3.87936800	2.20552900	-0.36144100
H	-2.60243700	1.58047500	-1.40285100
C	-3.17207700	-0.35637400	1.08212700
C	0.11502000	4.15336800	0.59593400
C	-3.30046600	1.29894700	-0.60049300
H	1.40681000	2.65223100	-0.35910000
H	0.25884900	4.84271000	-0.24199600
H	-0.89135700	4.26141900	1.00159900
H	0.83490400	4.44830800	1.37335600
Ga	0.76556600	-0.24278600	-0.01564300
Br	3.01520000	0.45236000	-0.64386700
Br	0.70873400	-1.54270100	2.01050900
Br	-0.35440200	-1.21643900	-1.92342500

GaBr₂-TS_{trans-a}

C	-3.38262000	0.95386100	-0.04159500
C	-1.92073100	1.31986900	0.12988600
C	-1.48500500	1.06842700	1.39209800
C	-2.57433400	0.47839400	2.24388800
C	-3.66812500	0.08848800	1.21565900
C	-1.07445900	1.98179800	-0.87613100
C	0.23656100	1.51789700	-1.12442800
H	-1.42382900	2.91365200	-1.33627500
H	-0.88110900	1.20008000	-1.86135200
H	-0.52787800	1.39469900	1.79769100
H	-2.22403600	-0.36350300	2.85178900
H	-2.91828900	1.24494400	2.95390300
H	-3.56914100	-0.97017500	0.95718800
H	-4.67830000	0.23998500	1.60078900
H	-3.98828900	1.87161300	-0.05962900
H	-3.58313200	0.42203400	-0.97812200
Ga	0.54574500	-0.27402700	-0.19469500
C	1.22766500	2.30940700	-1.92054600
C	2.20394000	3.00927100	-0.93535100
H	0.72331700	3.06701900	-2.53329200
H	1.79701100	1.65195200	-2.58570800
H	2.93254300	3.57529500	-1.52188300
H	1.67597600	3.70741000	-0.27886900
H	2.75104100	2.29040400	-0.31888200
Br	-0.49138700	-2.09411100	-1.24466100
Br	2.19477700	-0.48060400	1.44029800

GaBr₂-TS_{cis-a}

C	3.45861500	0.05948200	-0.07071500
C	2.12652600	0.61793400	-0.52678200
C	1.61835000	-0.07429600	-1.57737600
C	2.51561300	-1.21108600	-1.98485400
C	3.82847500	-0.95022600	-1.19285200
C	1.45895600	1.79926100	0.04617700
C	0.07782800	1.77561600	0.34419500
H	2.02039800	2.73661500	0.10653200
H	1.10941700	1.56620000	1.24212400
H	0.72969900	0.20765100	-2.14215100
H	2.04731300	-2.16907600	-1.71530200
H	2.66532900	-1.23913900	-3.06930200
H	4.25756500	-1.86940600	-0.78932900
H	4.57458500	-0.50556800	-1.85742000
H	4.21187500	0.84531300	0.06237800
H	3.34160900	-0.42965100	0.90673600
Ga	-0.69061600	-0.10607700	0.18520600
C	-0.72514300	2.99693600	0.67385400
C	0.02061900	4.32002100	0.87270100
H	-1.37911200	2.77537500	1.52762800
H	-1.42021000	3.07392700	-0.18220800
H	-0.70180800	5.11140600	1.08869900
H	0.71423000	4.27259400	1.72020300
H	0.57662400	4.61873300	-0.02203000
Br	-0.07837500	-1.63140300	1.85143900
Br	-2.42498200	-0.41741000	-1.34069700

GaBr₂-TS_{trans-b}

C	3.16098900	0.75416700	-0.49180100
C	1.76075400	1.04358700	-0.97252500
C	1.29797100	0.03619700	-1.77072400
C	2.33754500	-1.04645400	-1.96164800
C	3.37704500	-0.73833800	-0.85221700
C	0.97426300	2.28438700	-0.59935700
C	-0.46090300	1.89825900	-0.30566200
H	1.07881400	3.08328100	-1.34748100
H	1.36438200	2.69946500	0.34259300
H	0.40616600	0.10021900	-2.39601100
H	1.92309800	-2.05765800	-1.90289800
H	2.76439600	-0.94168300	-2.96895500
H	3.17502300	-1.35602200	0.02868500
H	4.40069000	-0.94582600	-1.16983100
H	3.85183100	1.41438000	-1.03932000
H	3.29819000	0.97154800	0.57345100
Ga	-0.33991200	-0.11266000	0.12090900
C	-1.51642100	2.81548800	-0.34504400
C	-2.92006300	2.54463800	0.11108300
H	-1.25587000	2.09318200	-1.37713300
H	-1.28408300	3.85106000	-0.61881600
H	-3.12812100	1.47861400	0.23139500
H	-3.03843800	3.03456800	1.08748000
H	-3.65247700	2.99409000	-0.56544200
Br	0.58211900	-0.45276400	2.25879900
Br	-1.93735900	-1.56090300	-0.81590000

GaBr₂-TS_{cis-b}

C	3.09578900	0.55163200	-0.55580400
C	1.69397800	0.99809600	-0.88846600
C	1.11831100	0.16717500	-1.80718700
C	2.06972400	-0.92593500	-2.24271600
C	3.18922600	-0.86866300	-1.17050700
C	1.01698500	2.20767700	-0.27278800
C	-0.40304000	1.84993000	0.09869000
H	1.10427000	3.09402800	-0.91643100
H	1.51281200	2.47658700	0.67338900
H	0.19940900	0.38873000	-2.35208500
H	1.59302000	-1.90772100	-2.32338700
H	2.44433400	-0.67740800	-3.24556300
H	3.79822900	1.25393000	-1.03163400
H	3.30614900	0.57841600	0.51935800
Ga	-0.40824700	-0.20872100	0.14164800
C	-1.42326800	2.78355300	0.32726400
C	-1.29916300	4.28120300	0.37403300
H	-2.37857900	2.37217000	0.66441400
H	-1.35111300	2.27196700	-0.82515000
H	-1.28319600	4.57148800	1.43337500
H	-0.38914700	4.65824700	-0.09706200
H	-2.17342200	4.75971500	-0.07630900
H	4.17671800	-1.07781200	-1.58629700
H	2.99619500	-1.61298900	-0.39158700
Br	-2.20299900	-1.30866200	-0.90053500
Br	0.62439100	-1.00411000	2.10021400

GaBr₂-TS_{trans-c}

C	3.10506400	0.83037100	-0.43122500
C	1.69430900	1.28789600	-0.71320400
C	1.15497700	0.60154700	-1.76479800
C	2.13746800	-0.38914500	-2.34584100
C	3.24184500	-0.47327200	-1.25923300
C	0.97384100	2.37752500	0.06067600
C	-0.45528900	1.91355800	0.26550000
H	1.03451100	3.34881100	-0.45003600
H	1.45832400	2.50131400	1.03890500
H	0.23307200	0.88123800	-2.27640100
H	1.68518400	-1.35652500	-2.58566300
H	2.51750300	0.02057000	-3.29246000
H	3.05935000	-1.33553100	-0.60985200
H	4.23928000	-0.59094900	-1.68710300
H	3.79211800	1.61599100	-0.78244800
H	3.30427700	0.69257300	0.63705500
Ga	-0.33100100	-0.13750700	0.13905000
C	-1.52947000	2.80110300	0.43630300
C	-2.98618800	2.41075200	0.46465300
H	-1.32109200	3.87288200	0.34508800
H	-0.99458600	2.43327800	1.48566200
H	-3.52849800	2.97462300	1.22872400
H	-3.41960000	2.67843500	-0.50704700
H	-3.13321100	1.33979700	0.62238300
Br	0.72278000	-1.03344100	2.05005800
Br	-1.94235000	-1.33729700	-1.07161000

GaBr₂-TS_{cis-c}

C	3.00047100	0.78323600	-0.54652800
C	1.58290300	1.13898100	-0.91861600
C	1.07733800	0.26067700	-1.83613300
C	2.10260400	-0.77838100	-2.23460700
C	3.20063200	-0.63240500	-1.14751600
C	0.81532300	2.32206000	-0.35677300
C	-0.53748900	1.82305300	0.12003700
H	0.69078200	3.10450200	-1.11939800
H	1.37135700	2.78268400	0.47032400
H	0.15852300	0.42388200	-2.40136700
H	1.69069400	-1.78983400	-2.30543000
H	2.47490400	-0.52335300	-3.23670500
H	3.05146900	-1.38219700	-0.36449000
H	4.20561600	-0.77406400	-1.54956600
H	3.66688600	1.52787300	-1.00979200
H	3.18229500	0.82965800	0.53330500
Ga	-0.37866600	-0.23188100	0.12351400
C	-1.60754700	2.66590200	0.45627400
C	-1.67204800	4.16176600	0.29671600
H	-0.89117300	2.27839600	1.40408100
H	-2.55059900	2.16696900	0.69532100
H	-2.19566500	4.61878500	1.14155300
H	-0.69089900	4.62778200	0.18554600
H	-2.26630600	4.37468500	-0.60165300
Br	-2.08906000	-1.47012100	-0.89750700
Br	0.71956500	-0.97407200	2.07842700

(GaBr₃)₂-TS_{trans-a}

H	-0.61883200	0.92778700	1.90629900
C	-1.48961900	1.77916400	1.79691200
C	-2.05410500	0.50691200	1.55029300
C	-1.07336900	4.28077000	-1.02809700
C	-0.09688800	4.85811100	0.03190000
C	-1.08863400	2.81546500	0.82439000
C	-1.72948800	3.12863200	-0.31478600
H	-1.57761300	2.14437700	2.82980200
C	0.10346500	3.72398700	1.07044700
H	-2.60941500	2.62152300	-0.69858800
H	-0.54316500	3.90321400	-1.91509400
H	-1.79867600	5.01783300	-1.39170000
H	0.84813600	5.19065600	-0.40472500
H	-0.55757200	5.72496900	0.51797100
H	0.14724400	4.09641700	2.10221100
H	1.03987900	3.17587900	0.89782300
Br	0.16648500	0.05640600	-1.45262300
Br	-1.93938400	-2.87095600	0.21811200
Br	-3.79872000	0.14148000	-1.67398700
C	-2.67457500	-0.21563200	2.70608900
C	-4.21900000	-0.15455500	2.54660500
H	-2.39127800	0.24715100	3.65981100
H	-2.36304800	-1.26492200	2.71606100
H	-4.67299700	-0.67657700	3.39372800
H	-4.58035400	0.87832900	2.54108700
H	-4.55488100	-0.64376300	1.62792700
Br	3.24252000	-2.42579700	-0.65887500
Br	3.61757100	1.64644600	-0.56300000
Br	1.52672500	-0.24116400	2.27089600
Ga	-2.01024000	-0.53121300	-0.23255700
Ga	2.38552900	-0.32054700	-0.01916700

(GaBr₃)₂-TS_{cis-a}

H	-1.10344800	1.53629900	1.12666700
C	-1.48905900	0.17988000	1.53524000
C	-2.20344100	1.38720000	1.68007500
C	-5.32799500	1.83559600	-0.40867000
C	-4.95302400	3.31738400	-0.13345900
C	-4.32113900	1.06285400	0.39950700
C	-3.31507500	1.84480600	0.82754300
H	-2.08162200	1.93411200	2.62083600
C	-3.49312300	3.28693500	0.39174700
H	-4.41244400	-0.00192500	0.59916900
H	-5.21370900	1.57012500	-1.46998800
H	-6.36220100	1.59678600	-0.13581200
H	-5.06266100	3.94882300	-1.01878200
H	-5.61292900	3.72257500	0.64117000
H	-3.31988600	4.00250900	1.20582400
H	-2.76787600	3.52917100	-0.39771400
Br	-2.07176800	0.02834000	-2.28866600
Br	0.90254200	-1.72328200	-0.44798700
Br	-2.79414700	-2.91092600	0.42747700

C	-0.62184700	-0.32645300	2.65100400
C	-0.47734900	0.51016600	3.92448900
H	0.36704600	-0.58891800	2.25701500
H	-1.07795200	-1.30531700	2.88433400
H	0.16870100	-0.02297700	4.62743200
H	-0.00434500	1.47712700	3.72088000
H	-1.43854900	0.68411900	4.42039600
Br	3.48606500	-0.17679500	2.06553900
Br	4.03236900	0.24945900	-1.96746600
Br	1.10963700	2.24059300	0.00143500
Ga	2.58585500	0.29377200	-0.10317700
Ga	-1.55779700	-0.95284900	-0.18523900

(GaBr₃)₂-TS_{trans-b}

H	0.75065300	0.51282900	1.89766200
C	1.15928900	-0.46655900	2.77619700
C	1.87141400	-0.06933300	1.64099900
C	2.33787300	3.99640000	-0.33579600
C	3.77800000	4.27727900	0.16864900
C	3.02295200	0.90345000	1.83552900
C	1.94360700	2.75142000	0.42238100
H	3.14444300	1.14865900	2.90322000
H	3.92378500	0.33129100	1.56368100
H	0.91981200	2.39021700	0.43475900
H	2.31172900	3.80185200	-1.41783700
H	1.65480500	4.83486100	-0.15482200
H	4.43340700	4.66347300	-0.61709200
H	3.74464600	5.02937400	0.96471100
H	4.88594400	3.06232900	1.65524200
H	4.89803500	2.37492100	0.03293100
Br	1.47731100	-3.36668900	0.05244500
Br	-0.28529300	-0.08102400	-1.48182400
Br	3.62428800	-0.44565300	-1.57623200
C	2.99298200	2.16565100	1.01270800
C	0.09238600	-1.49937900	2.89848300
C	4.27699000	2.93115400	0.75048700
H	1.42574600	0.03503600	3.71344900
H	-0.28030400	-1.87399800	1.94559800
H	0.54091000	-2.34681200	3.43761700
H	-0.73731100	-1.12472600	3.50463300
Br	-3.86245300	1.54619700	-1.59400800
Br	-3.22111600	-1.85889300	0.59364000
Br	-1.65714700	1.60297000	1.79387700
Ga	-2.50953800	0.30808000	-0.10402300
Ga	1.76389600	-1.00716400	-0.20107400

(GaBr₃)₂-TS_{cis-b}

H	0.84151800	0.19131400	1.98463900
C	1.52162600	-0.74695900	2.69279000
C	2.05562000	-0.08535800	1.58465700
C	1.67448100	4.08767400	-0.21123400
C	3.17011700	4.11295500	-0.62423400
C	3.03566900	1.05823400	1.71593900
C	1.55551900	2.80498900	0.57520900
H	3.20306800	1.34326900	2.76360500
H	3.98668300	0.61681000	1.37840700
H	0.59270700	2.40895500	0.88572700
H	0.99742300	4.11746900	-1.07282900
H	1.40597800	4.94565500	0.42351700
H	4.37086300	3.67979100	1.18183100
H	4.66635900	2.55308200	-0.14103800
Br	1.16513300	-3.23294600	0.08017300
Br	-0.20726300	0.14927700	-1.48375800
Br	3.67841700	-0.56434500	-1.66270000
C	2.75089600	2.28081000	0.87608600
C	1.70729000	-0.45927900	4.14874600
H	0.90024200	-1.61909100	2.47539600
C	3.88421800	3.14392700	0.35152900
H	2.29259600	-1.28926500	4.56821100
H	2.22839800	0.47554500	4.35687800
H	0.73687000	-0.46554000	4.65583600
Br	-1.63462600	0.78268500	2.15252100
Br	-3.63447300	1.99345100	-1.11159900
Br	-3.37464100	-1.98402300	-0.16320700
H	3.59697500	5.11985200	-0.60729600
H	3.27033900	3.73142100	-1.64564800
Ga	-2.46321400	0.20234500	-0.09011100
Ga	1.78702700	-0.94540000	-0.27325000

(GaBr₃)₂-TS_{trans-c}			
H	0.34874700	-0.90585400	1.46175700
C	1.57590800	-0.59882600	1.17633300
C	1.09304600	-0.25518500	2.43734300
C	5.96360700	-0.62763700	1.09770200
C	6.16326600	-2.10528800	0.66646600
C	2.33726000	-1.90026500	1.02079900
C	3.82254400	-1.62931200	0.94753500
H	2.11132100	-2.59473500	1.84465100
H	2.01725000	-2.39659400	0.09702100
H	4.03984500	0.31062800	1.88387500
H	6.21980600	0.07505400	0.29170900
H	6.58493100	-0.35077300	1.95804700
H	6.89568400	-2.21459200	-0.13806000
H	6.52622800	-2.68796700	1.52025000
H	4.57181200	-3.64763700	0.56271800
H	4.59709400	-2.56739500	-0.82772000
Br	2.27381100	-0.45372200	-2.43876700
Br	-0.91991300	1.30349500	-0.87999300
Br	2.58265400	2.77115900	0.02569200
C	4.48570800	-0.55319200	1.39800400
C	0.42877800	1.01688300	2.85026600
H	1.22111400	-0.99690000	3.23337600
C	4.75514800	-2.60847500	0.25973500
H	-0.54982000	0.82141600	3.30315300
H	1.05893200	1.46739500	3.62931900
H	0.32203400	1.73623800	2.03791100
Br	-3.57888600	0.89826600	2.00315300
Br	-4.30944600	-0.63071300	-1.72653200
Br	-1.53291700	-2.24704000	0.73854600
Ga	-2.80723200	-0.26158800	0.05646800
Ga	1.58942000	0.65090900	-0.45184100

(GaBr₃)₂-TS_{cis-c}			
H	-0.23875500	1.57208500	0.13333700
C	-1.51632800	1.12181600	0.17413200
C	-0.90297800	1.75094700	1.25951400
C	-5.85324900	1.27773200	0.66882200
C	-6.20327600	1.94348900	-0.68867100
C	-2.35764000	1.87807000	-0.82128500
C	-3.82120300	1.72327700	-0.46079500
H	-2.08546700	2.94005300	-0.88378800
H	-2.19521600	1.45553400	-1.82035200
H	-3.78763500	1.15925700	1.62929400
H	-6.15618000	0.22105600	0.69800700
H	-6.34599100	1.76532800	1.51856600
H	-7.03938600	1.45423200	-1.19579500
H	-6.48882100	2.98745800	-0.51881100
H	-4.74581500	2.79639200	-2.12757300
H	-4.87409400	1.04133900	-2.21005200
Br	-2.73845900	-1.77129000	-1.79301800
Br	0.96307400	-1.59056500	-0.59414600
Br	-1.86863100	-1.86359900	2.20487800
C	-4.34798900	1.38429700	0.72537700
C	-0.97462000	3.19278100	1.66941300
C	-4.89552700	1.89563300	-1.51810000
H	-0.34727900	1.11119500	1.94926900
H	0.03419000	3.59205300	1.81622400
H	-1.52418000	3.82354600	0.97009900
H	-1.47871300	3.22642700	2.64368400
Br	2.65886800	0.58557200	2.26975600
Br	4.76251200	-0.54301300	-1.06820600
Br	1.74224200	2.18446400	-1.20950800
Ga	-1.49041100	-0.92780600	0.04335500
Ga	2.75892700	0.24364100	-0.10767700

4			
C	-1.62990100	0.67735900	-1.59919000
C	-1.98158800	-0.64020800	-1.52393400
C	0.61154100	1.23684100	0.42457700
C	-0.37266600	2.27270200	0.87284500
C	-1.27201500	2.82113000	-0.25163200
C	-2.26453900	1.79353600	-0.82832700
C	1.73237100	0.78672900	0.15892500
Cl	-1.42252500	-1.05160000	1.90168400
Cl	0.92648200	-2.33309600	-0.78535700
H	-2.92442700	1.39634400	-0.04800300
H	-2.91319400	2.31492100	-1.55008300
H	-0.65203500	3.23910900	-1.05336500

H	-1.84686000	3.65273000	0.16786100
H	-0.98027700	1.86172300	1.68621200
H	0.22350100	3.08737900	1.29896300
C	3.06305500	0.27923700	-0.15149400
H	-0.85697500	0.96060500	-2.31737600
H	-1.58881200	-1.36168100	-2.23756800
H	-2.81727800	-0.96043500	-0.90205100
H	3.28017500	-0.59175500	0.47750900
H	3.09753800	-0.05316100	-1.19526600
C	4.11882100	1.39174700	0.09601500
H	4.12213600	1.71044000	1.14126300
H	5.10246900	0.97988700	-0.14427300
H	3.94091100	2.26016100	-0.54330200
Ga	-0.28337500	-0.79583400	0.09855500

5			
C	3.60401600	0.17775300	0.21347500
C	3.54010200	-1.15126300	-0.08649000
C	0.77498300	1.32537200	0.34759200
C	1.35242600	2.26877400	-0.66497000
C	2.86285100	2.52002400	-0.50103900
C	3.74538600	1.28935300	-0.78213500
C	0.08630900	1.04106000	1.33649000
Cl	0.75079000	-1.00811300	-2.14543300
Cl	0.69297400	-2.27742700	1.44487600
H	3.59110600	0.91421900	-1.80076800
H	4.79885100	1.60502900	-0.72273100
H	3.06733900	2.90807600	0.50381000
H	3.14172200	3.30953900	-1.20622000
H	1.12935700	1.89416200	-1.66960400
H	0.80376800	3.20927500	-0.54586300
C	-0.75090900	0.70733100	2.47717500
H	3.61008000	0.46523500	1.26726000
H	3.60288700	-1.90274900	0.69737000
H	3.62800000	-1.49778100	-1.11549700
H	-1.53221500	0.01000500	2.15257200
H	-0.15098200	0.21370200	3.25014000
C	-1.39959400	2.00307900	3.04011000
H	-2.03911800	2.47649700	2.29153900
H	-2.01643300	1.72136900	3.89754200
H	-0.64411800	2.71800900	3.37617800
Cl	-2.94731800	1.78891600	-0.80829500
C	-3.75716600	0.38224900	-1.62413200
C	-4.25965800	-0.65516000	-0.64254800
H	-3.03494800	-0.03684500	-2.32562400
H	-4.60455700	0.79732700	-2.17522000
H	-4.89440000	-0.21500400	0.12732000
H	-4.82213500	-1.41956400	-1.18442800
Cl	-2.91741800	-1.52934200	0.21141900
Ga	1.18483400	-0.81227400	-0.04653500

6			
C	1.52728300	2.17600200	0.24129300
C	1.36715500	0.67388600	0.08668200
Cl	-0.69812400	-1.97601400	-1.28156400
C	2.04308100	-0.37892200	0.23551900
C	2.54722500	-1.73622900	0.26834100
C	3.92019300	-1.93776900	-0.41913700
C	5.05491800	-1.28648200	0.39586900
C	4.83926800	0.18830000	0.57342200
C	4.50950500	0.77300200	1.73712900
Cl	-1.50715400	1.68380900	-1.60561800
H	5.12895200	-1.77618800	1.37443400
H	6.00261800	-1.46660900	-0.12685500
H	3.88350200	-1.52868200	-1.43482800
H	4.09085900	-3.01517500	-0.50872200
H	2.56733900	-2.10317900	1.30284700
H	1.78773700	-2.33348000	-0.26544700
H	0.56494000	2.62391600	0.50249200
H	2.20354100	2.32764700	1.08833400
H	4.97311700	0.80895700	-0.31352300
H	4.39921600	1.85025900	1.82469600
H	4.40629200	0.19875300	2.65562000
C	2.08622700	2.83118700	-1.03129500
H	3.06313900	2.41486600	-1.29314800
H	1.41080000	2.70025800	-1.88131700
H	2.20421600	3.90515800	-0.85666500
H	-4.26635600	-0.86800200	2.34783600
C	-4.33729900	-0.17301800	1.50963100
C	-3.27929300	0.90218400	1.57061500
H	-5.30941500	0.32986900	1.54820800
Cl	-4.27174900	-1.11996700	-0.01395800
H	-3.25289400	1.54095800	0.68785100

H	-3.35531400	1.49547700	2.48355300
Cl	-1.56038900	0.17630400	1.68935700
Ga	-0.50115500	0.05522900	-0.63043500

TS1

C	2.21521000	-0.33921300	0.28923300
C	4.08632700	0.11424400	1.80218100
C	4.70398700	0.13301300	0.59449500
Cl	-0.68474400	-1.73455700	-1.48650100
C	1.41401800	2.01854400	0.99726100
C	2.65514400	-1.64604300	-0.21235900
C	3.95340500	-1.58030700	-1.03359100
C	5.12157400	-1.10695700	-0.12883500
C	1.37414400	0.62436100	0.38916100
Cl	-1.29682900	1.95144000	-1.38638000
H	5.36342300	-1.89949600	0.58808100
H	6.00931200	-0.92425500	-0.74238400
H	3.82085400	-0.89686000	-1.87909000
H	4.17535400	-2.57105900	-1.44117500
H	2.75057500	-2.35837000	0.61704500
H	1.83141100	-2.00878300	-0.84638900
H	0.40015800	2.33926200	1.25529100
H	1.97158300	1.96297700	1.93730400
H	4.85341200	1.08772000	0.09179700
H	3.81132200	1.03043100	2.31328000
H	3.98239800	-0.80699900	2.37070800
C	2.04384500	3.05286800	0.04908000
H	3.07426900	2.78624300	-0.20486300
H	1.47075300	3.14316100	-0.87755800
H	2.05250200	4.03179700	0.53807600
Cl	-4.50446900	0.09227900	-0.28783400
C	-4.37234000	-0.82498800	1.24877500
C	-3.02522700	-1.48701100	1.41640200
H	-5.12266800	-1.62242800	1.22739000
H	-4.60171000	-0.14773600	2.07315400
H	-2.97979400	-2.08409100	2.32903700
H	-2.71614500	-2.07216500	0.55017300
Cl	-1.66419000	-0.23498000	1.66684900
Ga	-0.40689100	0.19350000	-0.54757900

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C	-1.59637500	0.62832900	-0.48678900
Cl	1.36970200	2.45584300	0.09420900
C	-2.26936500	-0.54822000	-0.74118300
C	-1.89221000	-1.93268400	-0.22387700
C	-2.88632000	-2.24554800	0.90993800
C	-4.27423200	-1.69192300	0.46927900
C	-4.03330500	-0.46732000	-0.37458000
C	-3.52759000	-0.58150300	-1.71284600
Cl	0.44681800	-0.45866100	2.23463200
H	-4.80083200	-2.43918900	-0.13677300
H	-4.89870700	-1.45179200	1.33287900
H	-2.56576300	-1.72266700	1.81680100
H	-2.94125300	-3.31332900	1.13772500
H	-1.96211200	-2.67033300	-1.03133400
H	-0.86608100	-1.96128900	1.14994800
H	-4.32235900	0.51239900	-0.00654100
H	-3.60418400	0.26866700	-2.38351100
H	-3.59597300	-1.54764700	-2.20797700
C	-2.11694200	1.99469100	-0.81947000
C	-2.39588700	2.83747500	0.45299600
H	-3.01905100	1.96894900	-1.43953600
H	-1.34240400	2.51562500	-1.39982600
H	-2.77359000	3.81880600	0.15333700
H	-3.14402500	2.36266900	1.09593000
H	-1.48910500	3.00052300	1.04342900
H	4.08039700	-2.12188200	-1.35294100
C	4.17670700	-1.08405100	-1.02991600
C	3.16626100	-0.18468900	-1.70203400
H	5.17034700	-0.71802200	-1.30887300
Cl	4.06039100	-1.03965400	0.76067900
H	3.16616400	0.83584400	-1.31894200
H	3.27685100	-0.19519100	-2.78776400
Cl	1.42429800	-0.79612100	-1.44291300
Ga	0.23892500	0.63763200	0.39363000

TS2

C	-2.53164400	-0.18644200	0.54151200
C	-1.62853000	0.89893900	0.13848600
C	-3.91754200	0.10863100	0.44362300

C	-2.81870400	0.66511800	-0.88547300
C	-4.73085800	-1.15197800	0.29264500
C	-2.33844800	-1.68638900	0.43826200
C	-3.68896400	-2.23282900	-0.08327400
Cl	1.44395700	2.23803000	-0.91628300
Cl	0.28791700	-1.08574500	-2.09524200
H	-5.54432700	-1.04647700	-0.43135800
H	-5.20048400	-1.35249300	1.26585500
H	-3.93091100	-3.20984200	0.33925700
H	-3.64343100	-2.35376200	-1.17033900
H	-1.47920000	-1.97796800	-0.16796800
H	-2.14011400	-2.01435000	1.46957000
H	-4.36752000	1.03383200	0.78601900
H	-3.34572100	1.59478500	-1.08133200
H	-2.70126200	0.00541100	-1.74027300
C	-1.72339800	2.26155300	0.85019600
C	-0.95389700	2.28101300	2.17676100
H	-2.77154000	2.52970500	1.03816100
H	-1.32351500	3.02900800	0.17843000
H	-1.06060200	3.25859600	2.65606000
H	-1.33104600	1.52307000	2.87299700
H	0.11863000	2.11293900	2.02845900
H	4.10922000	-1.29595500	2.07970000
C	3.95295700	-1.52663500	1.02454200
C	2.54313600	-1.99604800	0.75089000
H	4.62459800	-2.34324100	0.73914000
Cl	4.40309500	-0.08412700	0.05884200
H	2.32155400	-2.11692800	-0.30966400
H	2.31029800	-2.90716700	1.30481100
Cl	1.27904200	-0.77534400	1.37622500
Ga	0.20427500	0.51430200	-0.61892800

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C	-2.92806100	-1.55400000	0.09920600
C	-2.91564100	-0.19319300	-0.60538500
C	-3.85998700	0.63276900	-0.05218400
C	-4.62958500	-0.04163700	1.03046400
C	-4.28899900	-1.54145400	0.84423900
C	-2.18100700	0.08439600	-1.94795400
C	-1.38661000	0.77227700	-0.95189900
H	-2.74793900	0.68433400	-2.66049700
H	-1.80757900	-0.85208400	-2.36088000
H	-4.04139300	1.65942400	-0.35515200
H	-4.28704300	0.34989700	2.00333200
H	-5.69943000	0.19414200	0.97901000
H	-4.24772200	-2.08365300	1.79085100
H	-5.05642000	-2.01441200	0.22379000
H	-2.83308800	-2.38394200	-0.60544200
H	-2.10546100	-1.64493700	0.81912500
Cl	0.55689600	-2.10874900	-1.06103900
Cl	0.33395300	-0.10951800	2.09065400
C	-1.44438100	2.27953000	-0.88786000
C	-1.36364600	2.93296600	0.49499800
H	-2.30780600	2.65864700	-1.45047800
H	-0.56877700	2.59114000	-1.48363500
H	-1.32340400	4.02111900	0.39299200
H	-2.24035000	2.68455500	1.10404300
H	-0.47859400	2.61284200	1.05239500
H	2.85026600	1.03480400	1.45929000
C	3.36014800	1.35640800	0.55110600
C	4.56090500	0.51074700	0.19860000
H	3.61134600	2.41754700	0.59478900
Cl	2.05788700	1.28341100	-0.78708500
H	4.97574100	0.77417400	-0.77575300
H	5.31938800	0.69566300	0.96679500
Cl	4.19577700	-1.24554200	0.19994200
Ga	0.12879800	-0.25049500	-0.05989000

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C	1.71101100	-1.25751700	-0.72448400
C	1.64999300	-0.07666700	0.25278300
C	2.85195500	0.61071200	0.21199600
C	3.82954400	-0.02082200	-0.70260000
C	3.22784500	-1.41753300	-0.99898600
C	1.03939600	-0.20695100	1.77179100
C	0.31659500	0.61243000	0.82137500
H	1.61820800	0.26332500	2.56457600
H	0.79121100	-1.25320500	1.94046000
H	3.06272600	1.51369000	0.77943400
H	3.88711600	0.61427900	-1.60685700
H	4.84670900	-0.02179500	-0.29162600

H	3.43415000	-1.75585700	-2.01592000
H	3.65986700	-2.15174600	-0.31198600
H	1.25243500	-2.16894400	-0.33440900
H	1.17555100	-0.98746200	-1.64525200
Cl	-1.66053500	-2.29103800	0.37162300
Cl	-2.80530600	0.99169900	-0.94670900
C	0.31320800	2.13247100	1.00039800
C	0.42557600	2.94489700	-0.29297000
H	1.10347100	2.42599700	1.70552400
H	-0.62691100	2.38711400	1.50958600
H	0.36035400	4.01375500	-0.07114400
H	1.38345600	2.77086000	-0.79963100
H	-0.37644800	2.70508200	-0.99776600
Ga	-1.34978500	-0.19975600	0.04244000

DCE

C	0.71700500	-0.24954200	0.00020200
H	1.25515200	0.07502600	0.89148700
H	1.25523000	0.07528800	-0.89094100
C	-0.71700500	0.24954200	0.00020200
H	-1.25523000	-0.07528800	-0.89094100
H	-1.25515200	-0.07502600	0.89148700
Cl	-0.71700500	2.06400700	-0.00010300
Cl	0.71700500	-2.06400700	-0.00010300

E-10

C	2.52630900	1.24668500	0.44491300
C	1.40788000	1.16471100	-0.56016500
C	1.48406300	-0.00615100	-1.28378700
C	2.71784000	-0.80699400	-0.90740500
C	3.18682000	-0.15562000	0.42076000
C	0.33244200	2.21953900	-0.72599700
C	-0.84945700	1.83751300	0.15846900
H	0.01802800	2.28551800	-1.77334200
H	0.71411000	3.20035700	-0.42145200
H	0.93382300	-0.17205600	-2.21107400
H	2.53906500	-1.88364700	-0.82650100
H	3.45234400	-0.67654100	-1.71425900
H	2.83564100	-0.74281000	1.27386000
H	4.27462300	-0.09846500	0.49029200
H	3.20730900	2.03324500	0.08040100
H	2.19728400	1.56960100	1.43959100
Cl	-0.05695100	-1.01254600	2.09952900
Cl	-1.53249000	-1.71897300	-1.29723600
C	-2.09075300	1.51647000	-0.31162900
C	-3.29571200	1.25659000	0.52978800
H	-2.23791900	1.47413100	-1.39265100
H	-0.71683000	1.96627700	1.23410700
H	-4.02643700	2.05443600	0.33521400
H	-3.78363100	0.31853100	0.23991600
H	-3.07354700	1.24400600	1.60007700
Ga	-0.38161200	-0.50881300	0.04571500

Z-10

C	2.49346600	1.29249000	0.42445000
C	1.15470200	1.40511600	-0.25405000
C	1.08453400	0.56432900	-1.34390600
C	2.40803700	-0.14071400	-1.58232600
C	3.18853800	0.08725100	-0.26010900
C	0.03113700	2.30301800	0.22462100
C	-0.89481200	1.45898300	1.09203700
H	-0.50294400	2.73266100	-0.62743300
H	0.43415200	3.12680900	0.82381600
H	0.31583200	0.64720700	-2.11377900
H	2.30443600	-1.19650700	-1.85104700
H	2.89283400	0.34872900	-2.43835400
H	3.11205700	-0.79511400	0.38123300
H	4.25007500	0.27123600	-0.43543700
H	3.01800800	2.24241200	0.22969000
H	2.42097600	1.20704700	1.51522000
Cl	0.54393700	-1.72952000	1.69525300
Cl	-1.69200200	-1.50264500	-1.32408900
C	-2.21810900	1.19269600	0.86414100
C	-3.08132800	1.63805500	-0.26417600
H	-0.49260700	1.17299600	2.06545900
H	-2.72080100	0.59794400	1.62932500
H	-3.86692900	2.28637400	0.14964100
H	-2.55264200	2.19144100	-1.04254500
H	-3.59585600	0.78165200	-0.71540100
Ga	-0.33859600	-0.62823900	0.08760400

11

C	-2.93579600	0.19308500	1.53296600
C	-1.98748500	0.47546400	0.36998100
C	-2.58517900	0.13379700	-0.82144000
C	-3.94305400	-0.43468900	-0.62206800
C	-4.01800200	-0.71964300	0.89941700
C	-0.71390400	1.07933600	0.50206000
C	0.32093000	1.21274300	-0.47089300
H	-0.46896900	1.45577300	1.49937000
H	0.00556300	1.00902300	-1.50197800
H	-2.15843500	0.30477700	-1.80646300
H	-4.68172000	0.31817400	-0.95080400
H	-4.12409000	-1.30794300	-1.26237500
H	-5.01236100	-0.53523700	1.31019100
H	-3.77480800	-1.77049200	1.08408100
H	-2.43342200	-0.27821000	2.38357500
H	-3.36534900	1.13581700	1.89681600
Cl	0.59342100	-2.26146300	-1.12504800
Cl	3.01820800	-0.53735700	1.21848100
C	1.32803200	2.37025000	-0.32931400
C	0.71795100	3.69721900	-0.81091900
H	2.22979000	2.15469000	-0.91351600
H	1.64630500	2.45491300	0.71624600
H	1.45933900	4.49746100	-0.72534800
H	0.40760600	3.63965900	-1.85984000
H	-0.15496600	3.97474900	-0.20938200
Ga	1.35247900	-0.56511500	-0.08863500

GaCl₃-9

C	-2.30966600	-1.33281800	-0.36491100
C	-1.97496200	0.04202300	-0.92272100
C	-2.65944800	1.01423500	-0.26396400
C	-3.54212700	0.45157500	0.80962000
C	-3.56937700	-1.06737900	0.50027600
C	-0.96953500	0.26878200	-2.05814900
C	-0.12815100	0.84177300	-1.00931500
H	-1.32390100	0.95060900	-2.83651200
H	-0.63808800	-0.69015900	-2.45832100
H	-2.58599500	2.07718400	-0.46553700
H	-3.08462000	0.66058600	1.78842400
H	-4.53386000	0.91948100	0.82354300
H	-3.58004800	-1.67524900	1.40775800
H	-4.47179900	-1.30786900	-0.07178000
H	-2.48772200	-2.05077000	-1.17264400
H	-1.48626400	-1.73242600	0.23412400
Cl	1.17971000	-2.31975200	-0.84551200
Cl	3.08713000	0.69003400	-0.00378200
Cl	0.32841600	-0.41987700	2.18756300
C	0.01450600	2.32928100	-0.96371400
C	0.13732700	2.99942300	0.41018600
H	-0.73306000	2.83352100	-1.59228000
H	0.97799700	2.45322300	-1.49589700
H	0.34378800	4.06685900	0.28483500
H	-0.78961000	2.89317000	0.98357800
H	0.94843300	2.56456800	0.99906400
Ga	1.13980600	-0.33551600	0.12894300