

Supplementary material

Isomer-selective dative bond O→M (M = Si, Ge) for constructing new hemi-indigo photochromic systems

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Table S1. Selected geometrical parameters^a of the *E* isomers of silicon- and germanium-containing hemi-indigo **MY₂X-HI** and their stability (ΔE_{EZ} and ΔH_{EZ} , kcal/mol) relative to the *Z* isomer.

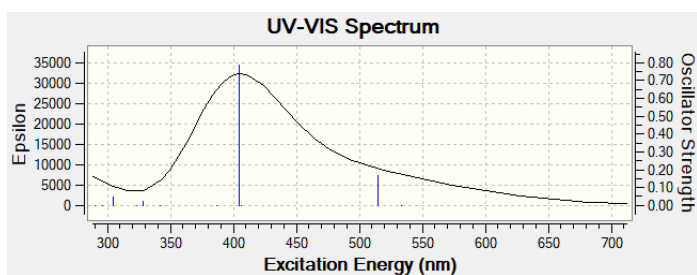
Compound	Method	Media	$d_{O \rightarrow M}$	d_{M-X}	η_a	ΔE_{EZ}	ΔH_{EZ}
SiF₃-HI	B3LYP	C ₆ H ₆	1.806	1.659	93	7.1	7.6
		CH ₃ CN	1.787	1.668	96	9.4	10.0
	B3PW91	C ₆ H ₆	1.801	1.655	93	8.2	8.7
		CH ₃ CN	1.783	1.663	96	10.4	11.1
SiCl₃-HI	B3LYP	C ₆ H ₆	1.792	2.237	96	0.6	0.9
		CH ₃ CN	1.766	2.278	98	3.6	4.0
	B3PW91	C ₆ H ₆	1.793	2.231	95	1.3	1.7
		CH ₃ CN	1.770	2.248	99	4.2	4.6
GeF₃-HI	B3LYP	C ₆ H ₆	1.926	1.784	92	12.7	13.1
		CH ₃ CN	1.906	1.793	96	14.9	15.4
	B3PW91	C ₆ H ₆	1.918	1.777	92	13.3	13.8
		CH ₃ CN	1.897	1.786	95	15.5	16.1
GeCl₃-HI	B3LYP	C ₆ H ₆	1.959	2.292	88	2.3	2.6
		CH ₃ CN	1.930	2.321	93	4.4	4.8
	B3PW91	C ₆ H ₆	1.958	2.269	87	2.5	2.9
		CH ₃ CN	1.929	2.294	92	4.6	5.0

^a Interatomic distances O→M and M-X ($d_{O \rightarrow M}$ and d_{M-X} , Å), and the degree of pentacoordination of the central atom M (η_a , %).

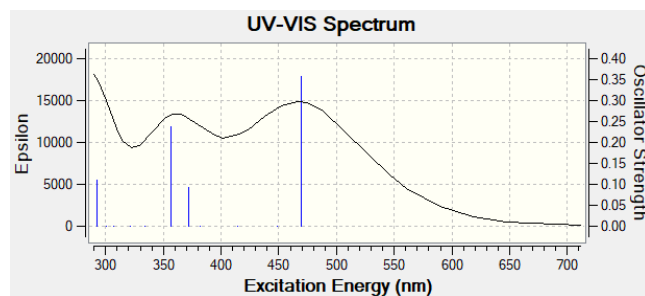
Table S2. Characteristics of first singlet-singlet electron transition (wavelength, λ /nm, and oscillator strength, f) of the absorption spectra of the *E* and *Z* isomers of **HI** and **MY₂X-HI**, and the difference in their absorption first band ($\Delta\lambda_{EZ}$ /nm).

Compound	Method	Media	λ_E	f_E	λ_Z	f_Z	$\Delta\lambda_{EZ}$
HI	exp.*	C ₆ H ₆	524		470		54
		CH ₃ CN	523		477		46
	TD-B3LYP/6-311+G(2d,p)// B3LYP/6-311G(d,p)	C ₆ H ₆	502	0.32	459	0.46	43
		CH ₃ CN	503	0.27	464	0.44	39
	TD-B3PW91/6-311+G(2d,p)// B3PW91/6-311G(d,p)	C ₆ H ₆	500	0.32	459	0.45	41
		CH ₃ CN	501	0.28	464	0.43	37
SiF₃-HI	TD-B3LYP/6-311+G(2d,p)// B3LYP/6-311G(d,p)	C ₆ H ₆	514	0.24	461	0.39	53
		CH ₃ CN	518	0.17	470	0.36	48
	TD-B3PW91/6-311+G(2d,p)// B3PW91/6-311G(d,p)	C ₆ H ₆	512	0.24	461	0.39	51
		CH ₃ CN	515	0.17	469	0.36	46
SiCl₃-HI	TD-B3LYP/6-311+G(2d,p)// B3LYP/6-311G(d,p)	C ₆ H ₆	522	0.21	463	0.40	59
		CH ₃ CN	525	0.14	470	0.37	55
	TD-B3PW91/6-311+G(2d,p)// B3PW91/6-311G(d,p)	C ₆ H ₆	518	0.21	463	0.40	55
		CH ₃ CN	522	0.14	470	0.37	52
GeF₃-HI	TD-B3LYP/6-311+G(2d,p)// B3LYP/6-311G(d,p)	C ₆ H ₆	527	0.21	462	0.37	65
		CH ₃ CN	532	0.15	470	0.35	62
	TD-B3PW91/6-311+G(2d,p)// B3PW91/6-311G(d,p)	C ₆ H ₆	525	0.21	462	0.38	63
		CH ₃ CN	529	0.15	470	0.35	59
GeCl₃-HI	TD-B3LYP/6-311+G(2d,p)// B3LYP/6-311G(d,p)	C ₆ H ₆	538	0.19	462	0.39	76
		CH ₃ CN	544	0.13	469	0.36	75
	TD-B3PW91/6-311+G(2d,p)// B3PW91/6-311G(d,p)	C ₆ H ₆	533	0.19	462	0.40	71
		CH ₃ CN	538	0.14	470	0.38	68

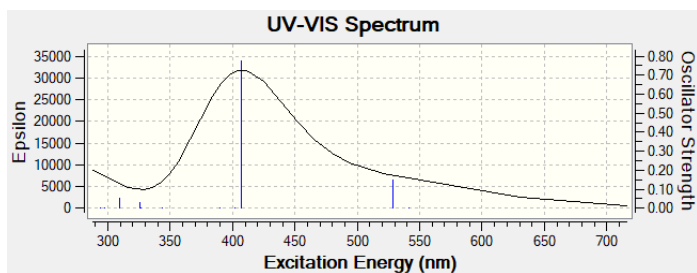
* M. Ikegami, T. Arai, Photoisomerization and Fluorescence Properties of Hemiindigo Compounds Having Intramolecular Hydrogen Bonding, Bull. Chem. Soc. Jpn. 76 (2003) 1783-1792. <https://doi.org/10.1246/bcsj.76.1783>



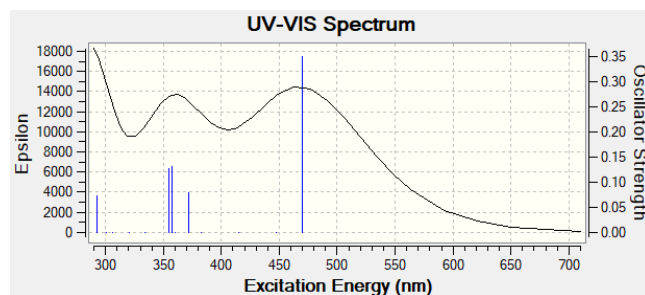
(E)-SiF₃-HI



(Z)-SiF₃-HI



(E)-GeF₃-HI



(Z)-GeF₃-HI

Figure S1. The TD-B3PW91/6-311+G(2d,p)//B3PW91/6-311G(d,p) UV-VIS absorption spectra of the hypervalent hemi-indigo **MY₂X-HI** in acetonitrile (C-PCM).

Computation information and geometries of the *E* and *Z* isomers of HI and MY₂X-HI

(*E*)-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -686.047597070 A.U.

C	-1.852998000	0.528344000	-0.000137000
C	-2.163010000	-0.848102000	-0.000065000
C	-2.866573000	1.489283000	-0.000017000
C	-3.492176000	-1.282188000	0.000185000
C	-4.184793000	1.064996000	0.000232000
C	-4.482519000	-0.310552000	0.000342000
H	-2.613492000	2.544477000	-0.000089000
H	-3.740642000	-2.337664000	0.000259000
H	-4.992962000	1.787490000	0.000366000
H	-5.521671000	-0.623966000	0.000564000
C	-0.405165000	0.661526000	-0.000287000
N	-1.005184000	-1.573460000	-0.000356000
C	0.111180000	-0.729045000	-0.000314000
O	0.250682000	1.716345000	-0.000314000
C	1.392325000	-1.206178000	-0.000147000
C	2.633057000	-0.519134000	-0.000022000
C	3.919407000	-1.080254000	0.000087000
C	4.841297000	-0.024222000	0.000324000
C	4.106799000	1.158027000	0.000206000
N	2.792423000	0.848775000	0.000034000
H	1.498544000	-2.288693000	-0.000127000
H	-0.955642000	-2.578660000	0.000555000
H	1.976287000	1.474588000	0.000082000
H	4.438684000	2.185310000	0.000267000
H	5.918724000	-0.096797000	0.000515000
H	4.135059000	-2.139061000	0.000060000

(*Z*)-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -686.042087956 A.U.

C	2.181819000	0.566969000	0.034179000
C	1.725227000	-0.762375000	-0.013502000
C	3.545051000	0.855120000	0.030287000
C	2.624103000	-1.825188000	-0.088403000
C	4.447388000	-0.197196000	-0.035399000
C	3.980654000	-1.519249000	-0.098703000
H	3.882747000	1.885631000	0.070874000
H	2.280920000	-2.852725000	-0.135203000
H	5.514133000	-0.004192000	-0.041448000
H	4.699098000	-2.330694000	-0.155795000
C	1.005236000	1.440951000	0.061285000
N	0.342762000	-0.793303000	0.043322000
C	-0.156891000	0.506959000	0.027718000
O	0.954249000	2.665191000	0.107054000
C	-1.443442000	0.929624000	-0.002865000
C	-2.641020000	0.154132000	0.006652000
C	-2.900615000	-1.201553000	0.232365000
C	-4.291367000	-1.397312000	0.138089000
C	-4.862487000	-0.167930000	-0.143449000

N	-3.866923000	0.750281000	-0.212496000
H	-1.549363000	2.011094000	-0.045498000
H	-0.185659000	-1.584526000	-0.288583000
H	-3.998348000	1.727717000	-0.421761000
H	-5.892955000	0.112447000	-0.296846000
H	-4.825642000	-2.326499000	0.268012000
H	-2.171714000	-1.956345000	0.484508000

(E)-SiF₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -1274.63484384 A.U.

C	-2.302598000	-0.221894000	-0.242718000
C	-2.901080000	0.994945000	0.185364000
C	-3.100456000	-1.333439000	-0.570054000
C	-4.291382000	1.112333000	0.298242000
C	-4.467620000	-1.210431000	-0.462545000
C	-5.049692000	0.004726000	-0.031285000
H	-2.638480000	-2.258499000	-0.895952000
H	-4.753187000	2.036198000	0.626234000
H	-5.111217000	-2.047647000	-0.706810000
H	-6.130181000	0.069019000	0.043151000
C	-0.899602000	-0.017714000	-0.218915000
N	-1.921589000	1.906154000	0.433346000
C	-0.675791000	1.332075000	0.187629000
O	0.007804000	-0.870120000	-0.581984000
C	0.507425000	2.036936000	0.151226000
C	1.812675000	1.598770000	-0.092373000
C	2.888719000	2.485433000	-0.298592000
C	4.031283000	1.730151000	-0.522248000
C	3.650401000	0.397045000	-0.413099000
N	2.317503000	0.290372000	-0.166948000
H	0.432476000	3.111775000	0.293214000
H	-2.067461000	2.848461000	0.757673000
H	4.261926000	-0.488148000	-0.481551000
H	5.029444000	2.084698000	-0.729121000
H	2.800358000	3.562364000	-0.287705000
Si	1.554012000	-1.316684000	0.185013000
F	1.634968000	-2.484171000	-0.951276000
F	0.772626000	-1.463313000	1.613611000
F	2.967142000	-1.869513000	0.866329000

(Z)-SiF₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -1274.61682585 A.U.

C	3.267640000	-0.697158000	-0.133427000
C	3.146911000	0.674847000	0.147101000
C	4.511729000	-1.323780000	-0.115928000
C	4.263907000	1.441186000	0.469300000
C	5.632245000	-0.566717000	0.196645000
C	5.497855000	0.798747000	0.488632000
H	4.590576000	-2.383010000	-0.337540000
H	4.178627000	2.498251000	0.694406000
H	6.613823000	-1.025990000	0.219346000
H	6.383151000	1.375453000	0.736187000
C	1.922902000	-1.216167000	-0.394880000
N	1.823768000	1.071918000	0.028943000

C	1.023006000	-0.027747000	-0.238927000
O	1.571032000	-2.351245000	-0.682998000
C	-0.321556000	-0.108811000	-0.362413000
C	-1.277122000	0.955351000	-0.296025000
C	-1.136641000	2.327496000	-0.420907000
C	-2.419062000	2.917213000	-0.326111000
C	-3.325002000	1.908072000	-0.141759000
N	-2.648794000	0.695558000	-0.127598000
H	-0.678319000	-1.119080000	-0.548066000
H	1.476120000	1.916616000	0.454970000
H	-4.396215000	1.941834000	-0.020274000
H	-2.654674000	3.968301000	-0.398536000
H	-0.213403000	2.849833000	-0.620851000
Si	-3.408807000	-0.804229000	0.236230000
F	-4.979384000	-0.576230000	0.214743000
F	-3.032593000	-1.923361000	-0.828485000
F	-2.998060000	-1.369362000	1.662620000

(E)-SiCl₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -2355.58810177 A.U.

C	-2.566479000	-0.214933000	-0.327468000
C	-3.304190000	0.885436000	0.194283000
C	-3.228308000	-1.391432000	-0.728718000
C	-4.696734000	0.823147000	0.323754000
C	-4.597193000	-1.443882000	-0.602491000
C	-5.317716000	-0.342750000	-0.080249000
H	-2.663001000	-2.227420000	-1.124134000
H	-5.262990000	1.656807000	0.721758000
H	-5.137897000	-2.334190000	-0.901959000
H	-6.396531000	-0.418327000	0.005528000
C	-1.205378000	0.161691000	-0.293487000
N	-2.439850000	1.888639000	0.505103000
C	-1.140239000	1.493329000	0.205089000
O	-0.192085000	-0.551010000	-0.710827000
C	-0.050603000	2.339001000	0.211288000
C	1.283700000	2.090217000	-0.118109000
C	2.204039000	3.124831000	-0.377382000
C	3.395955000	2.548151000	-0.790764000
C	3.212389000	1.172064000	-0.731602000
N	1.949414000	0.866041000	-0.330399000
H	-0.251090000	3.382712000	0.437313000
H	-2.695214000	2.784460000	0.888994000
H	3.924370000	0.393202000	-0.952158000
H	4.302053000	3.047206000	-1.097916000
H	1.973974000	4.176999000	-0.291028000
Si	1.385731000	-0.820378000	0.043209000
Cl	1.722965000	-2.269875000	-1.440728000
Cl	3.357274000	-1.325683000	0.998840000
Cl	0.439783000	-1.187974000	1.904682000

(Z)-SiCl₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -2355.58028748 A.U.

C	3.774829000	-0.713258000	-0.136991000
C	3.728072000	0.663418000	0.141847000

C	4.981556000	-1.408684000	-0.104611000
C	4.882156000	1.366304000	0.477817000
C	6.138776000	-0.715361000	0.222003000
C	6.077679000	0.655674000	0.512656000
H	5.003509000	-2.470763000	-0.325435000
H	4.853427000	2.426696000	0.701664000
H	7.092729000	-1.228937000	0.256644000
H	6.990876000	1.181829000	0.771216000
C	2.405820000	-1.156413000	-0.412505000
N	2.430852000	1.135034000	0.006959000
C	1.572447000	0.080156000	-0.266292000
O	1.994614000	-2.270635000	-0.704264000
C	0.225557000	0.071854000	-0.396399000
C	-0.664595000	1.192781000	-0.346633000
C	-0.409928000	2.546616000	-0.493345000
C	-1.636652000	3.242674000	-0.412643000
C	-2.622996000	2.315811000	-0.213325000
N	-2.056246000	1.048554000	-0.173806000
H	-0.177401000	-0.920853000	-0.577099000
H	2.124634000	1.991164000	0.442474000
H	-3.685207000	2.452968000	-0.094201000
H	-1.784791000	4.308568000	-0.498820000
H	0.555138000	2.984408000	-0.698721000
Si	-2.948595000	-0.417189000	0.140115000
Cl	-2.834830000	-1.682675000	-1.454513000
Cl	-4.898398000	0.059201000	0.462523000
Cl	-2.207247000	-1.367933000	1.782181000

(E)-SiCN₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -1253.43659600 A.U.

C	-2.466094000	-0.256428000	-0.295412000
C	-3.181517000	0.891087000	0.152046000
C	-3.151352000	-1.442957000	-0.624075000
C	-4.575306000	0.865401000	0.282155000
C	-4.520345000	-1.458398000	-0.497758000
C	-5.218708000	-0.311069000	-0.047902000
H	-2.603085000	-2.313793000	-0.964293000
H	-5.125080000	1.734166000	0.624023000
H	-5.079458000	-2.354339000	-0.741151000
H	-6.298872000	-0.359397000	0.039901000
C	-1.099740000	0.095537000	-0.286266000
N	-2.297679000	1.894865000	0.395844000
C	-1.005183000	1.453595000	0.131205000
O	-0.098725000	-0.661959000	-0.657787000
C	0.101181000	2.277435000	0.105165000
C	1.443790000	1.994579000	-0.158972000
C	2.399698000	3.003225000	-0.383175000
C	3.616949000	2.395021000	-0.657928000
C	3.406428000	1.027232000	-0.557741000
N	2.103871000	0.753545000	-0.263125000
H	-0.087045000	3.335090000	0.267878000
H	-2.534315000	2.814752000	0.732639000
H	4.127145000	0.232144000	-0.674020000
H	4.556883000	2.869467000	-0.893511000

H	2.182494000	4.061242000	-0.354803000
Si	1.493249000	-0.916691000	0.063317000
C	3.184384000	-1.479946000	0.843285000
N	4.157231000	-1.877290000	1.329974000
C	1.722327000	-2.234314000	-1.257214000
N	1.908223000	-3.054563000	-2.050719000
C	0.699081000	-1.195051000	1.748439000
N	0.215798000	-1.379369000	2.782896000

(Z)-SiCN₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -1253.40648691 A.U.

C	3.545058000	-0.692701000	-0.140399000
C	3.480257000	0.682480000	0.141019000
C	4.759431000	-1.373974000	-0.102970000
C	4.623092000	1.399249000	0.482832000
C	5.906468000	-0.666864000	0.230540000
C	5.827219000	0.702560000	0.522360000
H	4.795471000	-2.435148000	-0.325798000
H	4.580471000	2.458806000	0.707937000
H	6.866340000	-1.168827000	0.269386000
H	6.732582000	1.239565000	0.785892000
C	2.183824000	-1.150827000	-0.426667000
N	2.176304000	1.137321000	0.003391000
C	1.333358000	0.078673000	-0.281681000
O	1.783497000	-2.265742000	-0.724381000
C	-0.011379000	0.055321000	-0.425595000
C	-0.917221000	1.164150000	-0.377019000
C	-0.710747000	2.523302000	-0.524886000
C	-1.961792000	3.179810000	-0.432910000
C	-2.917293000	2.225634000	-0.226517000
N	-2.302267000	0.975881000	-0.193283000
H	-0.400096000	-0.941431000	-0.626692000
H	1.860838000	2.003501000	0.411005000
H	-3.984005000	2.323696000	-0.099316000
H	-2.143650000	4.240358000	-0.519239000
H	0.236732000	2.994936000	-0.736883000
Si	-3.116783000	-0.502977000	0.172068000
C	-4.894873000	-0.146529000	0.461766000
N	-6.016353000	0.052648000	0.649158000
C	-3.013025000	-1.732576000	-1.194096000
N	-2.950430000	-2.496107000	-2.058150000
C	-2.446329000	-1.321693000	1.677367000
N	-2.034967000	-1.827448000	2.630448000

(E)-SiNCS₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -2448.05902307 A.U.

C	2.994320000	0.513958000	-0.364132000
C	3.966541000	-0.497299000	-0.123972000
C	3.362828000	1.873021000	-0.363545000
C	5.304418000	-0.166729000	0.122772000
C	4.680196000	2.190426000	-0.125599000
C	5.636233000	1.174226000	0.114574000
H	2.619085000	2.640049000	-0.546402000
H	6.048266000	-0.932676000	0.308098000

H	4.998058000	3.226573000	-0.118359000
H	6.666474000	1.459855000	0.298955000
C	1.758631000	-0.148727000	-0.547580000
N	3.361300000	-1.713673000	-0.180568000
C	2.005988000	-1.549745000	-0.453495000
O	0.614746000	0.413831000	-0.823711000
C	1.152726000	-2.585617000	-0.771320000
C	-0.204592000	-2.570615000	-1.103298000
C	-0.864743000	-3.681123000	-1.665359000
C	-2.175312000	-3.312320000	-1.934628000
C	-2.315049000	-2.000801000	-1.496495000
N	-1.142416000	-1.527771000	-0.995847000
H	1.599820000	-3.574022000	-0.833709000
H	3.820580000	-2.601627000	-0.055967000
H	-3.197352000	-1.380340000	-1.507517000
H	-2.952496000	-3.910180000	-2.385183000
H	-0.393489000	-4.633768000	-1.860038000
Si	-1.000435000	0.080511000	-0.178900000
N	-2.675592000	-0.054211000	0.519785000
C	-3.700454000	-0.002770000	1.103347000
S	-5.100144000	0.048711000	1.876453000
N	-1.529452000	1.463751000	-1.103097000
N	-0.342508000	0.033282000	1.442917000
C	-0.002826000	0.163957000	2.572059000
C	-1.885533000	2.466431000	-1.623146000
S	0.463778000	0.316552000	4.079935000
S	-2.369908000	3.801054000	-2.333201000

(Z)-SiNCS₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -2448.04840994 A.U.

C	-4.447405000	0.574092000	-0.003659000
C	-4.482598000	-0.819590000	-0.183199000
C	-5.612043000	1.290721000	0.262768000
C	-5.679234000	-1.524752000	-0.079436000
C	-6.810534000	0.597753000	0.360530000
C	-6.831661000	-0.795139000	0.194099000
H	-5.570209000	2.366796000	0.395593000
H	-5.714526000	-2.600638000	-0.208398000
H	-7.733435000	1.127126000	0.567992000
H	-7.776145000	-1.322790000	0.279087000
C	-3.052589000	1.003234000	-0.134327000
N	-3.213662000	-1.295949000	-0.475105000
C	-2.293690000	-0.258551000	-0.402219000
O	-2.576996000	2.127967000	-0.055003000
C	-0.947520000	-0.286375000	-0.539396000
C	-0.114538000	-1.406296000	-0.854976000
C	-0.423513000	-2.652358000	-1.381573000
C	0.778947000	-3.376022000	-1.539523000
C	1.801286000	-2.571215000	-1.107377000
N	1.279653000	-1.359117000	-0.689535000
H	-0.482987000	0.685742000	-0.394021000
H	-2.960894000	-2.262109000	-0.337141000
H	2.861945000	-2.759817000	-1.059456000
H	0.888090000	-4.374954000	-1.934334000

H	-1.406961000	-2.986122000	-1.675926000
Si	2.231045000	-0.074760000	0.005836000
N	3.841804000	-0.594957000	0.020817000
C	5.022855000	-0.738971000	0.134543000
S	6.570535000	-0.956468000	0.271005000
N	2.083940000	1.340300000	-0.915553000
N	1.705421000	0.264846000	1.580039000
C	2.089547000	2.341872000	-1.565448000
C	1.419148000	0.504937000	2.713577000
S	2.080479000	3.658390000	-2.420947000
S	1.030087000	0.820815000	4.202068000

(E)-SiH₂OTf-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -1937.52893229 A.U.

C	-3.580765000	-0.711027000	-0.341129000
C	-4.323399000	-0.234651000	0.774311000
C	-4.064602000	-1.780822000	-1.117324000
C	-5.544897000	-0.820202000	1.128904000
C	-5.268831000	-2.347923000	-0.767525000
C	-5.995970000	-1.866240000	0.346978000
H	-3.494185000	-2.140773000	-1.965980000
H	-6.113977000	-0.463904000	1.979414000
H	-5.670589000	-3.173112000	-1.344028000
H	-6.941529000	-2.336170000	0.596224000
C	-2.398449000	0.065766000	-0.407473000
N	-3.645978000	0.795596000	1.346909000
C	-2.462561000	1.029182000	0.647583000
O	-1.452337000	-0.044086000	-1.296498000
C	-1.668350000	2.140612000	0.859126000
C	-0.490754000	2.555519000	0.231775000
C	0.034675000	3.860115000	0.337176000
C	1.147192000	3.939420000	-0.488805000
C	1.314039000	2.677480000	-1.055009000
N	0.338919000	1.833558000	-0.638747000
H	-2.039632000	2.854389000	1.590072000
H	-3.950047000	1.319770000	2.151514000
H	2.093488000	2.329898000	-1.714794000
H	1.779433000	4.796034000	-0.665533000
H	-0.399183000	4.646381000	0.938148000
Si	0.300125000	0.052435000	-0.959279000
H	0.218776000	-0.784763000	0.251599000
H	0.626483000	-0.330787000	-2.337478000
O	2.289603000	0.113773000	-0.629169000
C	3.740747000	-1.088884000	1.186986000
S	3.268891000	-1.043701000	-0.616504000
O	2.629551000	-2.327118000	-0.884909000
O	4.499666000	-0.722919000	-1.324087000
F	4.613746000	-2.073074000	1.391936000
F	4.296905000	0.063798000	1.548573000
F	2.664466000	-1.304410000	1.939661000

(Z)-SiH₂OTf-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -1937.50591983 A.U.

C	4.316301000	-1.201588000	0.023362000
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C	4.670618000	0.133186000	-0.239159000
C	5.283972000	-2.202854000	0.067801000
C	6.000319000	0.494440000	-0.442557000
C	6.610941000	-1.853805000	-0.140984000
C	6.954680000	-0.516228000	-0.388079000
H	4.995579000	-3.229525000	0.268180000
H	6.283207000	1.522522000	-0.638647000
H	7.386776000	-2.610301000	-0.111732000
H	7.997406000	-0.259269000	-0.544258000
C	2.865832000	-1.243919000	0.226403000
N	3.537245000	0.930610000	-0.271754000
C	2.420445000	0.174790000	0.059324000
O	2.145416000	-2.202222000	0.472229000
C	1.132241000	0.559840000	0.214756000
C	0.565977000	1.860141000	0.028140000
C	1.055527000	2.993824000	-0.605959000
C	0.060695000	3.995609000	-0.548982000
C	-1.015479000	3.465237000	0.115763000
N	-0.728877000	2.160655000	0.475344000
H	0.475217000	-0.255394000	0.508096000
H	3.582183000	1.928863000	-0.139989000
H	-1.964385000	3.911716000	0.371424000
H	0.122192000	4.993972000	-0.955468000
H	2.007787000	3.076648000	-1.107664000
Si	-1.822985000	1.161570000	1.404374000
H	-2.969831000	1.994583000	1.792669000
H	-1.132551000	0.446508000	2.486981000
O	-2.348561000	-0.026961000	0.271595000
C	-4.559348000	-0.754903000	-0.918745000
S	-3.327303000	-1.259517000	0.400275000
O	-4.005731000	-1.228641000	1.678418000
O	-2.659929000	-2.448898000	-0.068993000
F	-3.946478000	-0.665938000	-2.086313000
F	-5.501861000	-1.682935000	-0.974856000
F	-5.097151000	0.411349000	-0.600261000

(E)-GeF₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -3062.05808624 A.U.

C	-2.513320000	-0.192588000	-0.258197000
C	-3.140354000	1.001672000	0.188591000
C	-3.281450000	-1.327920000	-0.575542000
C	-4.530943000	1.073207000	0.334841000
C	-4.648791000	-1.250259000	-0.436362000
C	-5.259807000	-0.056856000	0.016230000
H	-2.796665000	-2.235116000	-0.917968000
H	-5.014972000	1.979768000	0.678730000
H	-5.270469000	-2.106429000	-0.671382000
H	-6.339794000	-0.028393000	0.115976000
C	-1.116240000	0.052542000	-0.269256000
N	-2.185436000	1.941701000	0.416344000
C	-0.923489000	1.411521000	0.143130000
O	-0.208597000	-0.783418000	-0.669848000
C	0.219039000	2.182131000	0.117031000
C	1.559311000	1.853109000	-0.112826000

C	2.574795000	2.817030000	-0.275550000
C	3.776978000	2.150285000	-0.475390000
C	3.493501000	0.790364000	-0.404663000
N	2.165214000	0.593860000	-0.202465000
H	0.069820000	3.247028000	0.276161000
H	-2.352922000	2.870735000	0.767908000
H	4.163880000	-0.052118000	-0.468623000
H	4.751458000	2.581506000	-0.646182000
H	2.409126000	3.884550000	-0.250064000
Ge	1.474885000	-1.132673000	0.135221000
F	1.633491000	-2.353629000	-1.110728000
F	0.652920000	-1.343943000	1.672622000
F	3.017942000	-1.680541000	0.848970000

(Z)-GeF₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -3062.03186286 A.U.

C	3.616742000	-0.721809000	-0.148636000
C	3.550384000	0.647375000	0.161578000
C	4.832167000	-1.402079000	-0.125312000
C	4.693276000	1.357674000	0.518535000
C	5.978550000	-0.701263000	0.222897000
C	5.897956000	0.661951000	0.543409000
H	4.869082000	-2.458495000	-0.369937000
H	4.649539000	2.412259000	0.765996000
H	6.938910000	-1.203087000	0.251313000
H	6.802861000	1.194118000	0.818249000
C	2.255609000	-1.175879000	-0.443567000
N	2.247083000	1.103884000	0.033070000
C	1.404597000	0.047190000	-0.272085000
O	1.859122000	-2.286612000	-0.764742000
C	0.059880000	0.026342000	-0.413837000
C	-0.850111000	1.128398000	-0.333968000
C	-0.662633000	2.498392000	-0.423211000
C	-1.924013000	3.131523000	-0.322825000
C	-2.870289000	2.152943000	-0.170043000
N	-2.230233000	0.924452000	-0.187563000
H	-0.339542000	-0.961770000	-0.633642000
H	1.929601000	1.955220000	0.469329000
H	-3.941052000	2.217908000	-0.056823000
H	-2.120884000	4.191848000	-0.373045000
H	0.279867000	2.992067000	-0.605679000
Ge	-3.075475000	-0.635515000	0.182699000
F	-4.769124000	-0.379522000	0.068287000
F	-2.643441000	-1.901890000	-0.898052000
F	-2.758190000	-1.253429000	1.755280000

(E)-GeCl₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -4143.07217138 A.U.

C	-2.743035000	-0.205433000	-0.352859000
C	-3.487158000	0.868369000	0.207813000
C	-3.390676000	-1.385259000	-0.763291000
C	-4.874837000	0.776691000	0.368825000
C	-4.755671000	-1.468559000	-0.606288000
C	-5.483654000	-0.392767000	-0.044862000

H	-2.818220000	-2.201438000	-1.188966000
H	-5.447123000	1.591209000	0.796857000
H	-5.285897000	-2.363304000	-0.911250000
H	-6.558609000	-0.490418000	0.064566000
C	-1.381637000	0.191061000	-0.348764000
N	-2.633872000	1.879881000	0.520736000
C	-1.330968000	1.519883000	0.182175000
O	-0.384037000	-0.505080000	-0.803653000
C	-0.277063000	2.407978000	0.192286000
C	1.071889000	2.243056000	-0.139743000
C	1.941988000	3.327392000	-0.371087000
C	3.173112000	2.818079000	-0.762346000
C	3.059651000	1.432327000	-0.727599000
N	1.804517000	1.066954000	-0.363948000
H	-0.528772000	3.435516000	0.441851000
H	-2.896668000	2.760137000	0.934135000
H	3.813136000	0.689887000	-0.938821000
H	4.057839000	3.368280000	-1.043826000
H	1.657150000	4.365623000	-0.278284000
Ge	1.329422000	-0.736361000	0.047906000
Cl	1.716496000	-2.208621000	-1.520818000
Cl	0.295265000	-1.149175000	1.949977000
Cl	3.353639000	-1.170207000	1.036542000

(Z)-GeCl₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -4143.06367438 A.U.

C	4.050890000	-0.732427000	-0.126164000
C	4.057053000	0.650156000	0.126524000
C	5.233347000	-1.468759000	-0.103261000
C	5.241315000	1.318552000	0.426276000
C	6.420044000	-0.810130000	0.187170000
C	6.412061000	0.567532000	0.451822000
H	5.214348000	-2.534918000	-0.303713000
H	5.253669000	2.383379000	0.629492000
H	7.356303000	-1.355795000	0.213346000
H	7.347920000	1.066348000	0.682007000
C	2.662321000	-1.132986000	-0.366529000
N	2.774416000	1.163712000	0.007477000
C	1.875535000	0.134076000	-0.231443000
O	2.207652000	-2.238325000	-0.627405000
C	0.527638000	0.169607000	-0.347159000
C	-0.334204000	1.310100000	-0.306435000
C	-0.060043000	2.666776000	-0.415651000
C	-1.279798000	3.374353000	-0.352070000
C	-2.284420000	2.452412000	-0.202200000
N	-1.726390000	1.188854000	-0.180502000
H	0.091190000	-0.813069000	-0.506962000
H	2.507338000	2.038075000	0.431683000
H	-3.349171000	2.594574000	-0.109997000
H	-1.414141000	4.443579000	-0.418347000
H	0.914321000	3.099900000	-0.582959000
Ge	-2.695268000	-0.354087000	0.098671000
Cl	-4.748746000	0.162349000	0.323221000
Cl	-2.502825000	-1.688985000	-1.557198000

Cl -2.030842000 -1.364435000 1.857102000

(E)-GeCN₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -3040.90382387 A.U.

C -2.664828000 -0.229702000 -0.328737000
C -3.386052000 0.877356000 0.195369000
C -3.336198000 -1.407182000 -0.706920000
C -4.775834000 0.820439000 0.353386000
C -4.703162000 -1.455714000 -0.554093000
C -5.408444000 -0.347573000 -0.027774000
H -2.779976000 -2.247689000 -1.105987000
H -5.332122000 1.659331000 0.754419000
H -5.252165000 -2.346872000 -0.835194000
H -6.485680000 -0.418063000 0.080134000
C -1.294008000 0.134991000 -0.330853000
N -2.512897000 1.880748000 0.477971000
C -1.215519000 1.482062000 0.159651000
O -0.309227000 -0.594788000 -0.747201000
C -0.146023000 2.348369000 0.143532000
C 1.207492000 2.156890000 -0.168174000
C 2.095661000 3.222783000 -0.400883000
C 3.339154000 2.691695000 -0.726486000
C 3.212535000 1.312054000 -0.652727000
N 1.936093000 0.968441000 -0.327474000
H -0.382029000 3.387203000 0.359698000
H -2.757560000 2.775705000 0.870357000
H 3.969157000 0.557504000 -0.808091000
H 4.240286000 3.226695000 -0.983684000
H 1.819767000 4.266090000 -0.346611000
Ge 1.449390000 -0.817548000 0.075434000
C 3.251654000 -1.246818000 0.879860000
N 4.261066000 -1.543029000 1.362420000
C 1.652140000 -2.203290000 -1.271634000
N 1.822511000 -3.031590000 -2.058610000
C 0.553886000 -1.173343000 1.767324000
N 0.030216000 -1.394309000 2.773358000

(Z)-GeCN₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -3040.88642411 A.U.

C 3.850059000 -0.702731000 -0.149772000
C 3.814532000 0.671376000 0.142975000
C 5.047274000 -1.413264000 -0.101193000
C 4.969576000 1.356953000 0.507886000
C 6.206059000 -0.737255000 0.255121000
C 6.155702000 0.631216000 0.558417000
H 5.060895000 -2.473092000 -0.332901000
H 4.948930000 2.415151000 0.742392000
H 7.152859000 -1.262745000 0.303234000
H 7.069857000 1.143607000 0.840064000
C 2.482001000 -1.125433000 -0.458125000
N 2.524724000 1.159151000 -0.008901000
C 1.660165000 0.121534000 -0.312112000
O 2.059791000 -2.228575000 -0.771442000
C 0.316425000 0.133421000 -0.466790000

C	-0.562972000	1.261934000	-0.411535000
C	-0.324829000	2.621571000	-0.541382000
C	-1.560394000	3.301870000	-0.447154000
C	-2.538309000	2.361122000	-0.256375000
N	-1.946198000	1.109880000	-0.242202000
H	-0.096214000	-0.851274000	-0.680153000
H	2.223151000	2.026637000	0.406550000
H	-3.603665000	2.477797000	-0.131575000
H	-1.721079000	4.366709000	-0.523091000
H	0.633986000	3.073863000	-0.745217000
Ge	-2.838640000	-0.438833000	0.149740000
C	-4.663564000	0.000932000	0.488003000
N	-5.769058000	0.257774000	0.695074000
C	-2.775231000	-1.689815000	-1.297036000
N	-2.733738000	-2.435382000	-2.176867000
C	-2.106036000	-1.298756000	1.692433000
N	-1.666205000	-1.807630000	2.630097000

(E)-GeNCS₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -4235.50347436 A.U.

C	3.095576000	0.346069000	-0.356803000
C	4.046925000	-0.493767000	0.284079000
C	3.451177000	1.644143000	-0.769025000
C	5.351626000	-0.048776000	0.527692000
C	4.736468000	2.074476000	-0.530784000
C	5.671912000	1.229641000	0.112750000
H	2.722077000	2.279923000	-1.258031000
H	6.080671000	-0.682970000	1.017916000
H	5.043377000	3.068841000	-0.833660000
H	6.676940000	1.599725000	0.285911000
C	1.880923000	-0.381935000	-0.420540000
N	3.459043000	-1.684631000	0.574409000
C	2.129476000	-1.670195000	0.155293000
O	0.777970000	0.025506000	-0.973244000
C	1.334701000	-2.796381000	0.150585000
C	-0.000963000	-2.991265000	-0.218235000
C	-0.577705000	-4.267418000	-0.375043000
C	-1.900378000	-4.100715000	-0.764729000
C	-2.131731000	-2.730592000	-0.809514000
N	-1.000863000	-2.048089000	-0.493856000
H	1.828040000	-3.718610000	0.446369000
H	3.898569000	-2.450693000	1.059394000
H	-3.046185000	-2.204953000	-1.037561000
H	-2.626159000	-4.867482000	-0.987872000
H	-0.047499000	-5.196584000	-0.223107000
Ge	-0.984497000	-0.177138000	-0.259162000
N	-2.789821000	-0.160600000	0.396612000
C	-3.744127000	0.270910000	0.948188000
S	-5.061251000	0.805001000	1.679303000
N	-1.523252000	0.793238000	-1.738372000
N	-0.341587000	0.344639000	1.405285000
C	-0.195086000	1.236934000	2.183600000
C	-1.619887000	1.842171000	-2.293675000
S	0.036966000	2.367046000	3.268314000

S -1.791201000 3.199544000 -3.093980000

(Z)-GeNCS₃-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -4235.49014718 A.U.

C -4.679597000 0.380955000 0.718599000
C -4.766479000 -0.215463000 -0.551395000
C -5.813642000 0.542490000 1.511542000
C -5.984024000 -0.679864000 -1.042825000
C -7.033000000 0.089914000 1.027125000
C -7.105135000 -0.517607000 -0.235396000
H -5.732465000 1.007636000 2.488463000
H -6.058400000 -1.148749000 -2.017485000
H -7.932723000 0.200140000 1.621553000
H -8.065141000 -0.871433000 -0.597143000
C -3.273531000 0.717848000 0.955065000
N -3.520806000 -0.228031000 -1.159088000
C -2.564046000 0.264693000 -0.283011000
O -2.756655000 1.252196000 1.926817000
C -1.222541000 0.359605000 -0.433480000
C -0.435947000 0.018769000 -1.578856000
C -0.786758000 -0.208771000 -2.903475000
C 0.392100000 -0.473529000 -3.634577000
C 1.445481000 -0.409891000 -2.756279000
N 0.956542000 -0.101937000 -1.503109000
H -0.720181000 0.762276000 0.443603000
H -3.300976000 -0.850996000 -1.920249000
H 2.502248000 -0.557068000 -2.915551000
H 0.466856000 -0.678336000 -4.692050000
H -1.782405000 -0.132954000 -3.313509000
Ge 2.003184000 -0.035832000 0.003555000
N 3.692899000 -0.306278000 -0.576277000
C 4.838849000 -0.382177000 -0.220715000
S 6.357980000 -0.496962000 0.152944000
N 1.834384000 1.539467000 0.872212000
N 1.501008000 -1.266272000 1.227335000
C 2.037120000 2.721939000 0.820330000
C 1.423927000 -2.437427000 1.478611000
S 2.261882000 4.275457000 0.838577000
S 1.285743000 -3.946557000 1.890915000

(E)-GeH₂OTf-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -3725.01695713 A.U.

C -3.718248000 -0.731538000 -0.272475000
C -4.423636000 -0.263220000 0.867882000
C -4.233744000 -1.784056000 -1.050233000
C -5.641756000 -0.840457000 1.247194000
C -5.435135000 -2.343939000 -0.677140000
C -6.126049000 -1.870203000 0.462808000
H -3.689378000 -2.137130000 -1.918787000
H -6.184062000 -0.490559000 2.117665000
H -5.861262000 -3.156211000 -1.254529000
H -7.070029000 -2.332865000 0.731150000
C -2.524245000 0.032025000 -0.366747000
N -3.718656000 0.750117000 1.436311000

C	-2.549504000	0.985877000	0.708606000
O	-1.616890000	-0.091319000	-1.283531000
C	-1.753637000	2.091640000	0.936677000
C	-0.580071000	2.545403000	0.322979000
C	-0.075943000	3.855120000	0.467661000
C	1.038364000	3.977033000	-0.352502000
C	1.224826000	2.736073000	-0.959005000
N	0.259437000	1.871336000	-0.568632000
H	-2.124252000	2.779308000	1.693180000
H	-3.993777000	1.262731000	2.258395000
H	2.010471000	2.417669000	-1.626481000
H	1.656631000	4.849085000	-0.501489000
H	-0.525182000	4.617849000	1.087490000
Ge	0.277575000	0.008279000	-0.924382000
H	0.221645000	-0.851258000	0.323073000
H	0.644124000	-0.338128000	-2.346965000
O	2.437302000	0.171619000	-0.552365000
C	3.826704000	-1.082888000	1.281154000
S	3.388732000	-0.997783000	-0.528719000
O	2.732038000	-2.270636000	-0.821192000
O	4.647114000	-0.711175000	-1.206802000
F	4.677481000	-2.086419000	1.491490000
F	2.732251000	-1.289298000	2.012757000
F	4.397315000	0.053475000	1.675003000

(Z)-GeH₂OTf-HI, B3PW91/6-311G(d,p), cpcm(CH₃CN), E = -3724.99606924 A.U.

C	4.516306000	-1.242016000	0.052211000
C	4.865738000	0.074323000	-0.296523000
C	5.488716000	-2.232746000	0.170009000
C	6.195369000	0.428089000	-0.514457000
C	6.815427000	-1.891432000	-0.052570000
C	7.154264000	-0.571442000	-0.386259000
H	5.203852000	-3.245324000	0.436450000
H	6.474811000	1.442212000	-0.777061000
H	7.594751000	-2.640111000	0.032483000
H	8.196766000	-0.319805000	-0.552392000
C	3.064427000	-1.279258000	0.246667000
N	3.728716000	0.860882000	-0.391123000
C	2.613037000	0.121261000	-0.018975000
O	2.347734000	-2.224007000	0.551140000
C	1.321186000	0.508284000	0.098087000
C	0.747454000	1.787632000	-0.181284000
C	1.240099000	2.885820000	-0.878331000
C	0.234908000	3.876054000	-0.907286000
C	-0.851447000	3.374138000	-0.230966000
N	-0.555650000	2.104357000	0.213373000
H	0.665419000	-0.290833000	0.435591000
H	3.766514000	1.865837000	-0.323952000
H	-1.811094000	3.824082000	-0.025216000
H	0.293151000	4.846212000	-1.377704000
H	2.201168000	2.946580000	-1.366256000
Ge	-1.717491000	1.109713000	1.250873000
H	-2.965435000	1.931134000	1.493917000

H	-1.017490000	0.374987000	2.374035000
O	-2.167039000	-0.226192000	0.003521000
C	-4.464097000	-0.963323000	-1.028597000
S	-3.181656000	-1.386097000	0.267736000
O	-3.809870000	-1.220572000	1.566530000
O	-2.602246000	-2.652504000	-0.118428000
F	-3.908974000	-0.983315000	-2.229882000
F	-5.432164000	-1.866677000	-0.969234000
F	-4.963819000	0.239877000	-0.786419000