

Supporting Information C

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Quantum chemical calculations.

On the basis of the molecular structures of **1**, **5**, **7**, **8**, **9**, **10** determined in the solid state, and in the case of $[\text{TbbSn}(\text{NH}_3)\text{IrH}_2(\text{PMe}_3)_3]^+$, based on the molecular structure of **5** (while Ge was exchanged against Sn) the geometries of the bimetallic complexes were optimized using the programme Orca4.2.1¹⁻² along with BP86,³⁻⁴ Grimme's dispersion correction and Becke-Johnson damping (D3BJ).⁵ The basis sets employed were def2-TZVP for Ge, Sn, Ir, N, O, as implemented in ORCA4.2.1, and def2-SVP on all other elements.⁶⁻⁹ For all calculations, tight or very tight convergence criteria were applied for optimisations and SCF convergence, respectively; as gridsizes "grid6" and "finalgrid7" were selected. Absence of imaginary frequencies on this level of theory confirmed local minima on the PES. Analyses of the electronic structures were performed using NBO7, plots were generated using ChemCraft.¹⁰

On the basis of optimized structures NMR chemical shifts were computed for **5**, **8** and **10** at SO-ZORA level with ADF,^{11, 12-13} (PBE density functional, basis sets: TZ2P for Ir, Sn, N, O and TZP for P, C, H).¹⁴ The obtained ¹¹⁹Sn NMR shieldings were converted to chemical shifts (δ , in ppm) relative to the shieldings of SnMe_4 ($\sigma_{\text{ref}} = 2867$ ppm) calculated at identical computational level. ($\delta_{\text{calc}} = \sigma_{\text{ref}} - \sigma_{\text{sample}}$)

Case Study Cation 4: Geometry Optimisation

Cation **4** [TbbSn-Ir(H)(PMe₃)₃]⁺ was optimised starting from the experimental X-ray structure with BP86-D3BJ, M06-2X and ω B97X-D3BJ and def2-SVP basis sets (def2-TZVP and ECP on Sn and Ir) with suitable RI approximations (RI/ RIJCOSX) in ORCA4.2.1. The structural features from the optimised structures differed from those experimentally observed. The most obvious deviations are documented and summarised in Table SI-X and clearly BP86 fails in reproducing the experimental structure. Single point calculations on the BP86-optimised structure with ω B97X-D3BJ (def2-SVP basis sets and def2-TZVP and ECP on Sn and Ir) and vice versa revealed the bent BP86 structure to be energetically favored in both cases, however much more pronounced in BP86 (by 17.2 kcal mol⁻¹) than in ω B97X-D3BJ (by 2.7 kcal mol⁻¹). Depictions were created using ChemCraft programme.

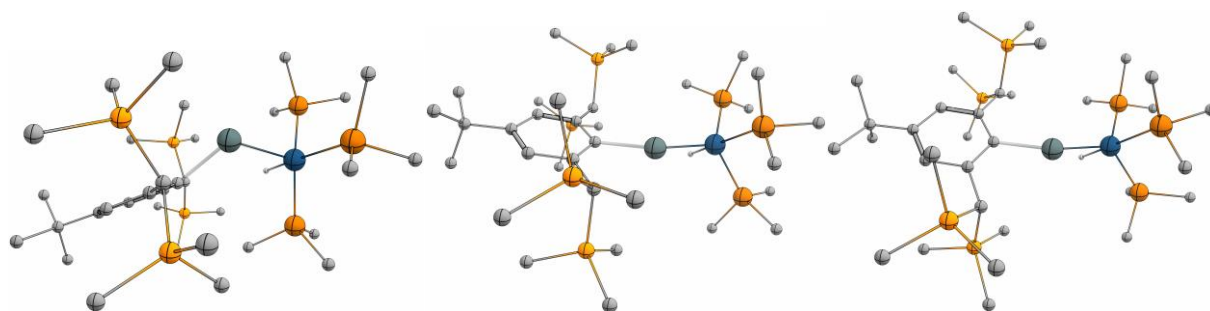


Figure SI 1. Depictions of optimised structures of cation **4** with (from left to right) BP86-D3BJ, M06-2X and ω B97X-D3BJ. Hydrogen atoms (except for the Ir-Hydride) were omitted for the sake of clarity.

Table SI 1.

	Sn-Ir [Å]	C-Sn-Ir [°]	P _{eq} -Ir-P _{eq} [°]
BP86-D3BJ	2.606	119.8	154.5
M06-2X	2.464	166.8	118.3
ω B97X-D3BJ	2.391	161.5	107.4
experimental	2.414	159.2	112.4

Case Study Model Cation $[\text{MeSn-Ir(H)(PMe}_3)_3]^+$: Geometry Optimisation

The model cation $[\text{MeSn-Ir(H)(PMe}_3)_3]^+$ was optimised with BP86-D3BJ and ω B97X-D3BJ and def2-SVP basis sets (def2-TZVP and ECP on Sn and Ir) with suitable RI approximations (RI/ RIJCOSX) in ORCA4.2.1 starting from the modified (Tbb \rightarrow Me) experimental structure. With each functional structures were optimised both freely without any constraints and once with the Ir-Sn-Me angle being constrained to the starting value (ca. 159°).

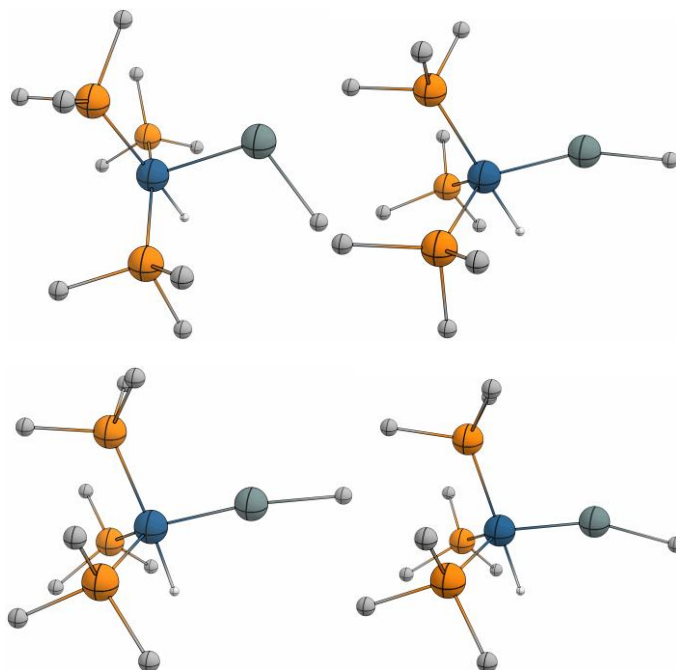


Figure SI 2. Depictions of optimised structures of cation $[\text{MeSn-Ir(H)(PMe}_3)_3]^+$ Top left: BP86-D3BJ + free optimisation; top right: BP86-D3BJ + constrained optimisation; bottom left: ω B97X-D3BJ + free optimisation; bottom right: ω B97X-D3BJ + constrained optimisation. Hydrogen atoms (except for the Ir-Hydride) were omitted for the sake of clarity.

Table SI 2.

	entry	mode	Sn-Ir [Å]	C-Sn-Ir [°]	$P_{\text{eq}}\text{-Ir-}P_{\text{eq}}$ [°]
BP86-D3BJ	1	free	2.561	107.8	154.7
BP86-D3BJ	2	constrained	2.437	159.2	110.8
ω B97X-D3BJ	3	free	2.374	172.0	112.6
ω B97X-D3BJ	4	constrained	2.376	159.2	113.2
experimental (for 4)			2.414	159.2	112.4

To elucidate the bonding situation in **4**, NBO/NLMO analysis and EDA-NOCV analysis on the constrained (159.2° C-Sn-Ir angle) optimised structure (entry 4, Table SI 2) of model cation $[\text{MeSn-Ir(H)(PMe}_3)_3]^+$ was performed. Wavefunction for NBO analysis was obtained from a singlepoint calculation with ω B97X-D3BJ and def2-SVP basis set and def2-TZVP + ECP basis set on Sn and Ir.

EDA NOCV analyses were performed using SCM ADF 2022 on the same structure (entry 4, Table SI 2) of $[\text{MeSn-Ir(H)(PMe}_3)_3]^+$ using ω B97X functional and TZ2P basis set on all elements and „good“ numerical quality.¹⁵⁻¹⁸ Depictions were created using the ADF GUI.

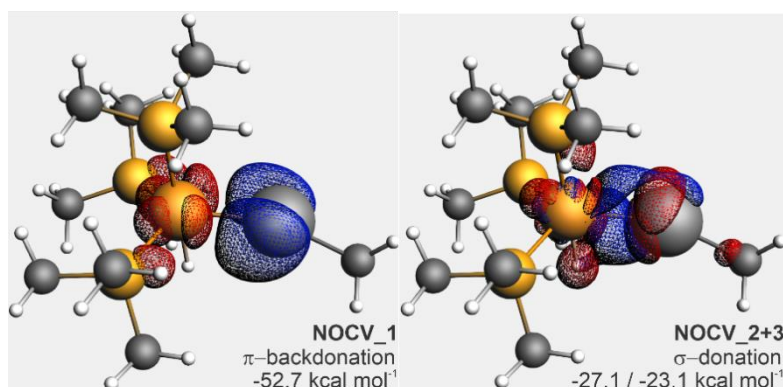
Along the lines of a EDA-NOCV bonding analyses study of (Schrock vs. Fischer-type) carbyne-transition metal complexes by Frenking, several electronic configurations of the constituting fragments $\{[\text{Ir}(\text{H})(\text{PMe}_3)_3]$ and $[\text{MeSn}]^+\}$ have been considered.¹⁹ Table Table SI-3 summarises the relevant ΔE_{orb} contributions to the total fragment interaction energy.

Table SI 3.

	dative	dative-el. shared	electron-shared (triple)	electron shared (double)
fragmentation	$[\text{Ir}(\text{H})(\text{PMe}_3)_3]$ // $[\text{SnMe}]^+$	$[\text{Ir}(\text{H})(\text{PMe}_3)_3]^+$ // $[\text{SnMe}]$	$[\text{Ir}(\text{H})(\text{PMe}_3)_3]^+$ // $[\text{SnMe}]$	$[\text{Ir}(\text{H})(\text{PMe}_3)_3]$ // $[\text{SnMe}]^+$
electron configuration $[\text{Ir}(\text{H})(\text{PMe}_3)_3]$	singlet	doublet	quartet	triplet
electronic configuration $[\text{SnMe}]$	singlet	doublet	quartet	triplet
$\Delta E_{\text{orb}} [\text{kJ mol}^{-1}]$	-502.0	-415.2	-898.1	-783.0

This analysis reveals that the fragment interaction definitively includes dative components as the pure electron sharing interactions are much higher. As already observed by Frenking and coworkers, the mixed [dative+electron sharing] partition into fragments with electronic doublet states gives low ΔE_{orb} interaction values. Despite this observation we consider the partition into $[\text{Ir}(\text{H})(\text{PMe}_3)_3]$ // $[\text{SnMe}]^+$ to be the most reasonable description of the system.

The results of the ETS-NOCV analysis (excerpt of the output file) along the respective fragmentation leading to consideration of DATIVE (see Table SI-3) interactions is shown below. The respective difference density plots for the three leading NOCV 1-3 are also shown in the main manuscript (Figure 4).



=====
ETS-NOCV-decomposition: taken restricted fragments
=====

Orbital Interaction Energy Contributions from each NOCV pair (in kcal/mol)

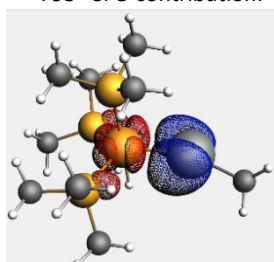
- 1 -52.77632
- 2 -27.06847
- 3 -23.78326
- 4 -10.43697
- 5 -1.35970
- 6 -2.60291
- 7 -1.90649

8 -2.18450
9 -1.30047
10 0.29247
Total sum: -129.579873812074 (kcal/mol)

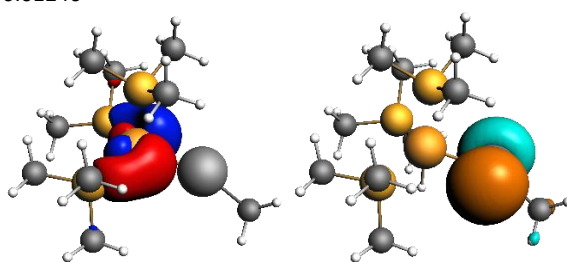
=====
SFO decomposition of Delta rho k (major contributions):
=====

Threshold for a NOCVs energy (in kcal/mol) is 2.00000000000000
Threshold for an individual SFO contribution is 1.00000000000000E-002

1 NOCV eigenvalues: -0.87007 0.87007, sum from all SFOs: -0.77328E-14
Corresponding Delta E k: -52.77632 (kcal/mol)
102 SFO contribution: -0.64311
781 SFO contribution: 0.61738
791 SFO contribution: 0.01440
793 SFO contribution: 0.01246

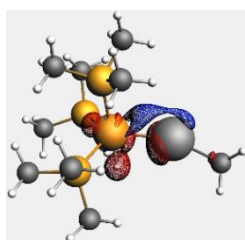


NOCV_1 (diff density)

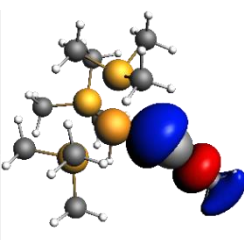


SFO102 [Ir(d)-type] SFO781 [Sn(p*)-type]

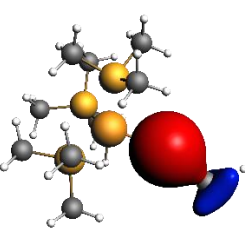
2 NOCV eigenvalues: -0.51231 0.51231, sum from all SFOs: 0.12985E-13
Corresponding Delta E k: -27.06847 (kcal/mol)
103 SFO contribution: 0.26761
782 SFO contribution: 0.17831
780 SFO contribution: -0.16972
777 SFO contribution: -0.10446
100 SFO contribution: -0.07455
101 SFO contribution: -0.07452
98 SFO contribution: -0.04241
794 SFO contribution: 0.01177



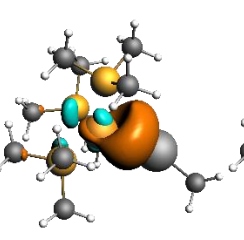
NOCV_2 (diff density)



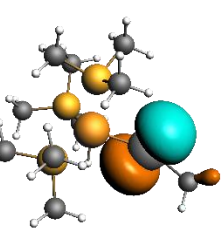
SFO780 [Sn(sp)-type]



SFO777 [Sn(s)-type]

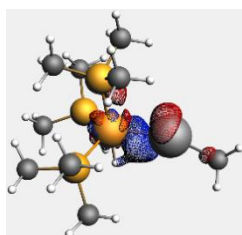


SFO103 [Ir(s*)-type]

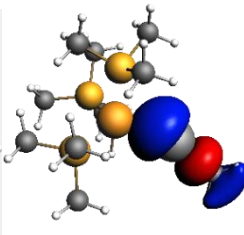


SFO782 [Sn(p*)-type]

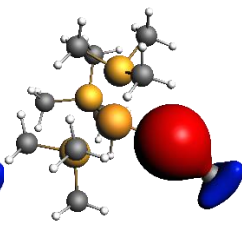
3 NOCV eigenvalues: -0.47433 0.47433, sum from all SFOs: -0.74147E-14
Corresponding Delta E k: -23.78326 (kcal/mol)
103 SFO contribution: 0.22581
780 SFO contribution: -0.19775
777 SFO contribution: -0.07680
100 SFO contribution: -0.07501
782 SFO contribution: 0.06770
98 SFO contribution: -0.01284
101 SFO contribution: 0.01064



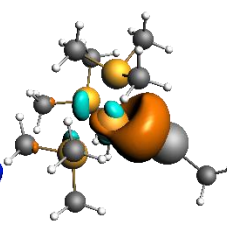
NOCV_3 (diff density)



SFO780 [Sn(sp)-type]



SFO777 [Sn(s)-type]



SFO103 [Ir(s*)-type]

Selected NLMOs

[TbbGeBrIrH(PMe₃)₃] (1)

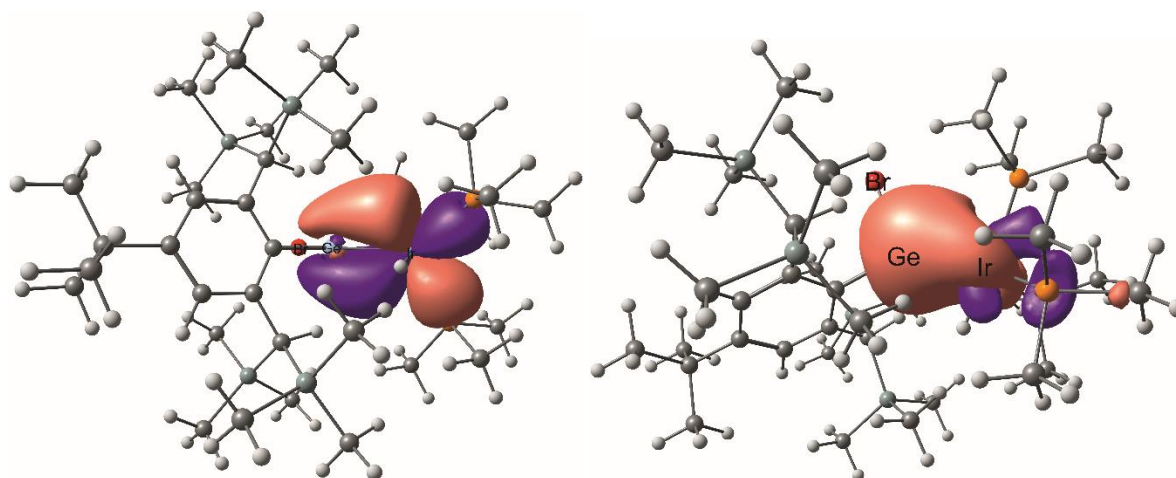


Figure SI 3. NLMO 107 and 108 of **1** showing the σ -donation Ge to Ir and π -donation into the empty p-orbital at Ge.

NLMO 107 13.3% Ge (p-orb.) 81.3 % Ir (d-orb.)

NLMO 108 75.0% Ge (s-orb.) 15.3% Ir (d-orb.)

[TbbGe(NH₂)IrH(PMe₃)₃][BAR^f₄] (5)

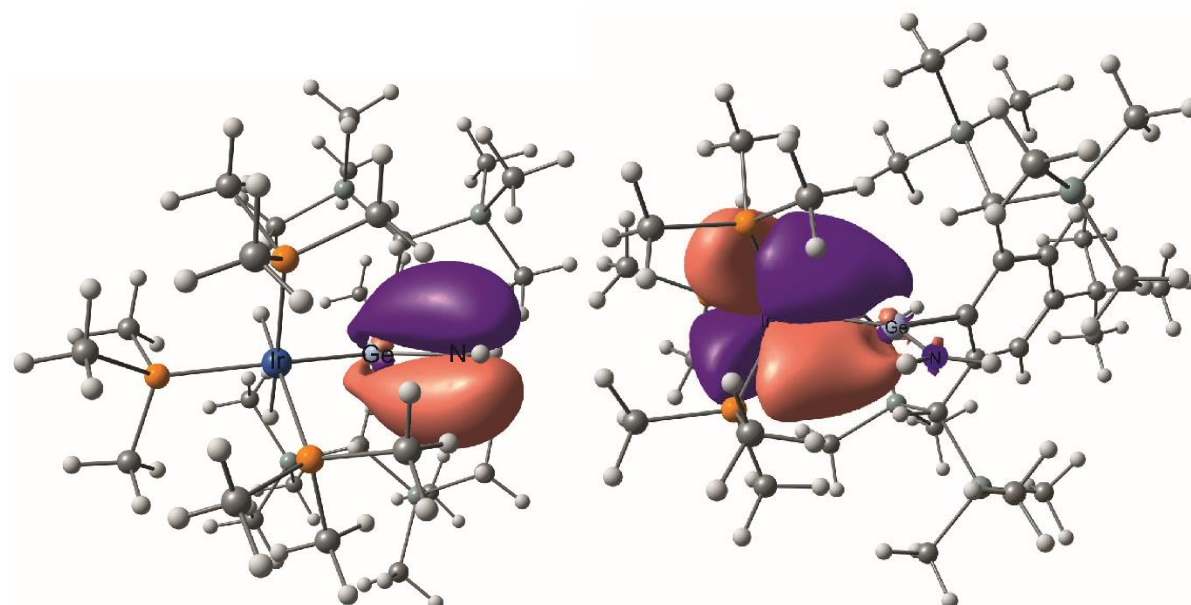


Figure SI 4. NLMO 88 and 94 of **5** showing the π -donation into the empty p-orbital at Ge.

NLMO 88 86.5% N (p-orb.) 12.3 % Ge (p-orb.)

NLMO 94 76.1% Ir (d-orb.) 7.7% Ge (s,p-orb.)

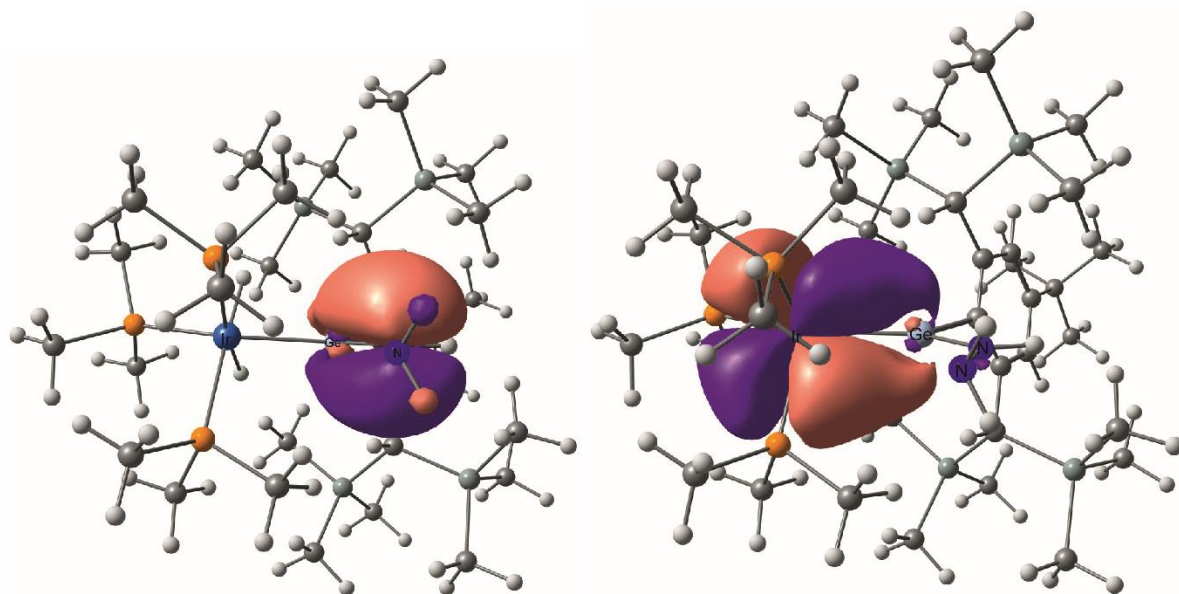
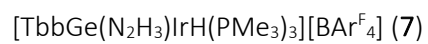


Figure SI 5. NLMO 89 and 96 of **7** showing the π -donation into the empty p-orbital at Ge.

NLMO 89	86.4% N (p-orb.)	11.3 % Ge (p-orb.)
NLMO 96	94.3% Ir (d-orb.)	2.3% Ge (p-orb.)

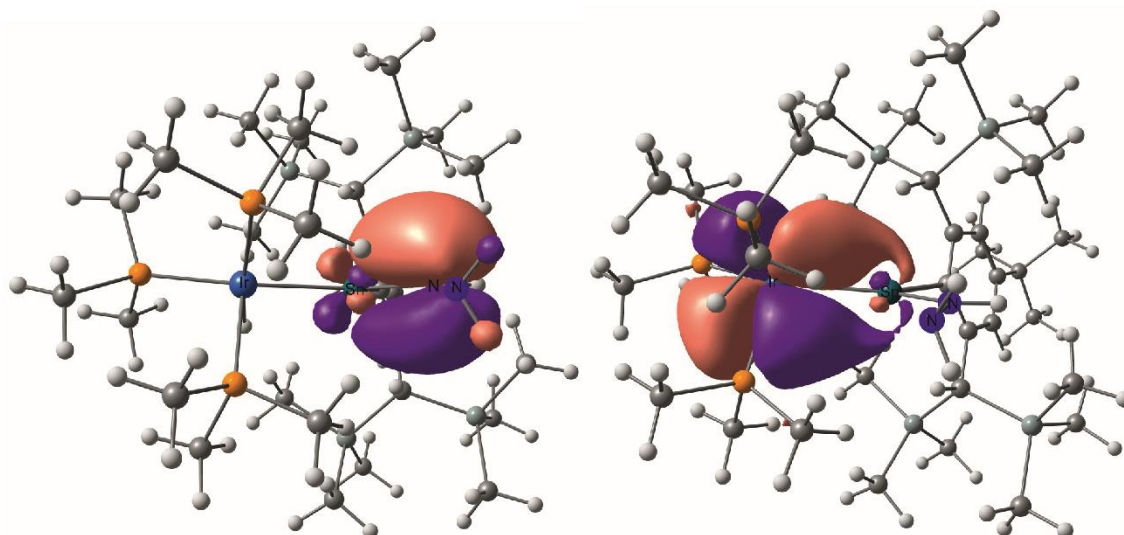
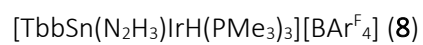


Figure SI 6. NLMO 84 and 90 of **8** showing the π -donation into the empty p-orbital at Sn.

NLMO 84	89.1% N (p-orb.)	8.1 % Sn (p-orb.)
NLMO 90	95.5% Ir (d-orb.)	0.9% Sn (p-orb.)

Results of NMR-calculations

[TbbSn(NH₃)IrH₂(PMe₃)₃]⁺

TOTAL NMR SHIELDING TENSOR (ppm)

CARTESIAN AXIS REPRESENTATION

total shielding tensor

1943.485 -161.793 971.588

-161.793 2874.768 314.568

971.588 314.568 1662.471

isotropic = 2160.241

PRINCIPAL AXIS REPRESENTATION

Principal components:

765.187 2747.610 2967.927

Principal Axis System:

-0.641 0.737 -0.216

-0.161 -0.404 -0.900

0.750 0.542 -0.378

Compound **8**.

TOTAL NMR SHIELDING TENSOR (ppm)

CARTESIAN AXIS REPRESENTATION

total shielding tensor

2814.513 -121.314 626.941

-121.314 2580.408 529.263

626.941 529.263 1190.630

isotropic = 2195.184

PRINCIPAL AXIS REPRESENTATION

==== Principal components:

811.701 2735.524 3038.325

Principal Axis System:

-0.302 0.264 -0.916

-0.292 -0.940 -0.174

0.907 -0.215 -0.361

Compound **10**.

TOTAL NMR SHIELDING TENSOR (ppm)

CARTESIAN AXIS REPRESENTATION

total shielding tensor

2728.819 215.589 993.812

215.589 2291.944 -492.702

993.812 -492.702 1251.170

isotropic = 2090.644

PRINCIPAL AXIS REPRESENTATION

Principal components:

582.856 2459.727 3229.349

Principal Axis System:

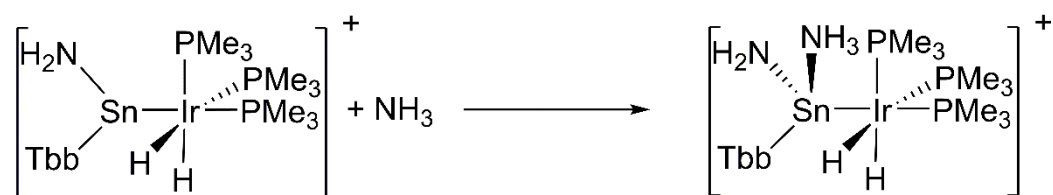
-0.426 0.166 0.890

0.300 0.953 -0.035

0.854 -0.252 0.456

Approximated thermochemical data

Approximated thermochemical data for NH₃ adduct formation of [TbbSn(NH₂)IrH₂(PMe₃)₃]⁺

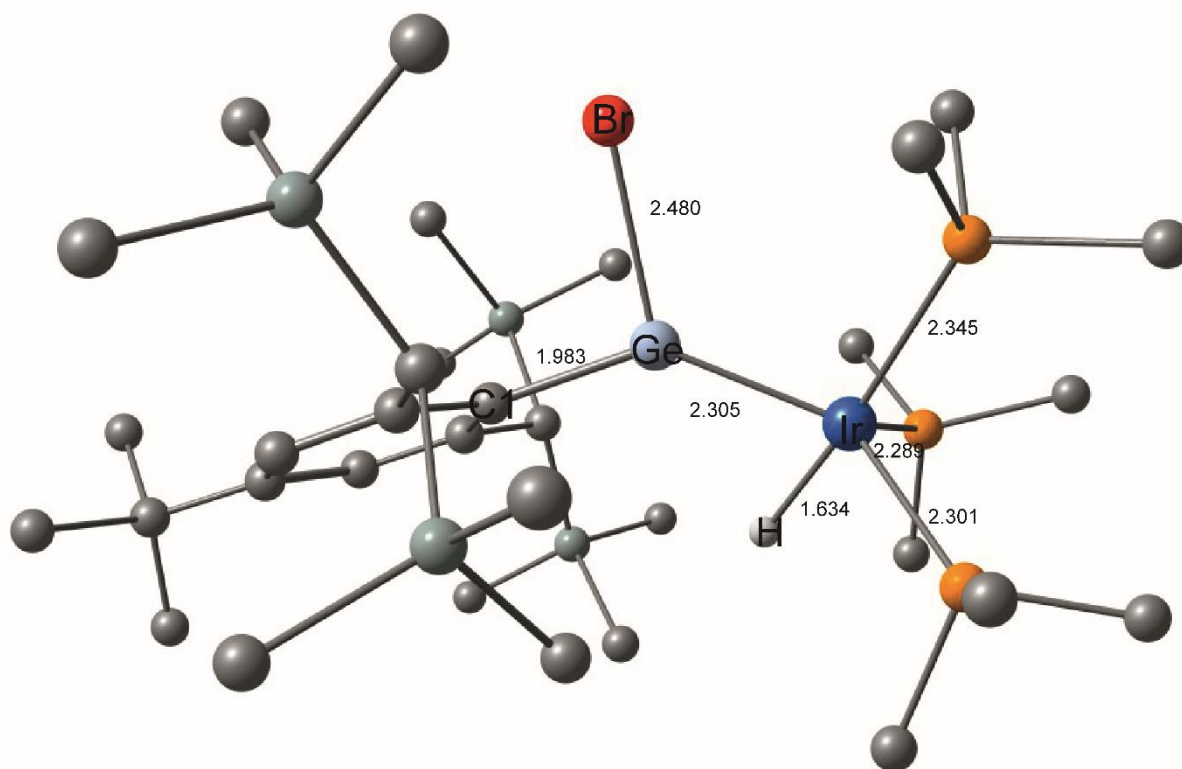


Scheme S1. NH₃-adduct formation of [TbbSn(NH₂)IrH₂(PMe₃)₃]⁺.

Evaluated based on results of DFT calculations: $\Delta H_R = -15.6$ kcal/mol, $\Delta G_R = -3.94$ kcal/mol

Coordinates and selected geometrical parameters for the optimized structures
All hydrogen atoms attached to carbon atoms and all isopropyl substituents on the ligand attached to the Group 14 element are omitted in the following plots for clarity; distances in Å, angles in degree.

Compound 1.



Angle C1-Ge-Ir: 138.5°.

Coordinates x, y, z

120

Coordinates from ORCA-job bp86optfreq_hnumac

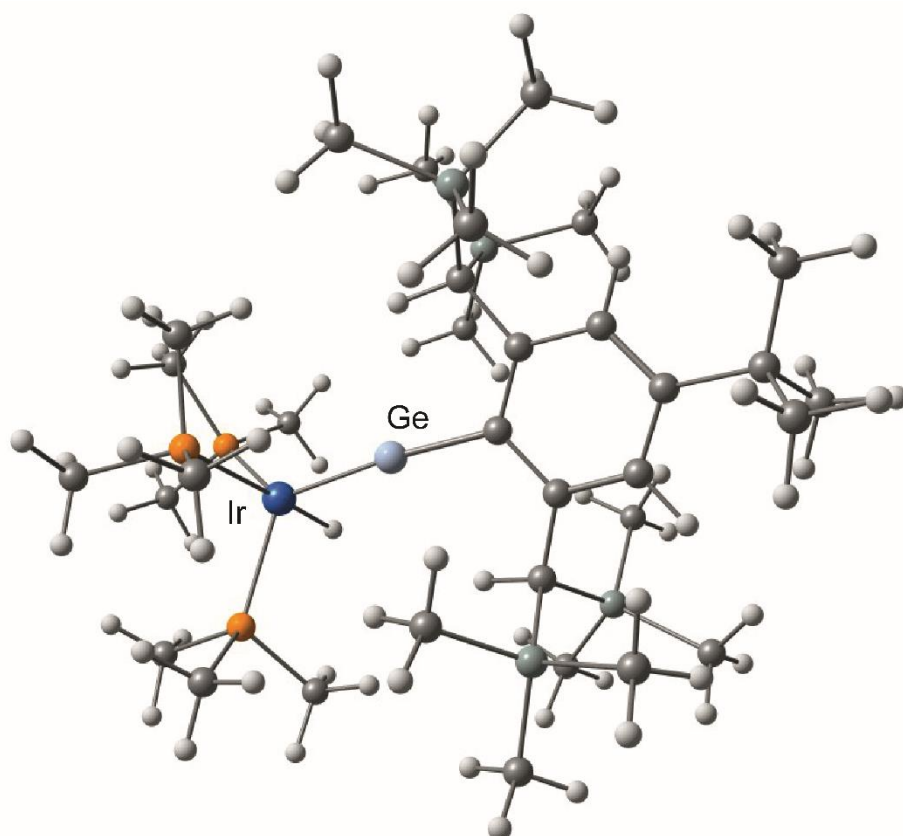
Br	5.65897513326988	3.94654745257127	-3.33247035645271
Ir	3.34581319997774	3.80362693178554	0.19730219768307
Ge	3.51060784092318	3.81515726849952	-2.10153571029795
P	3.56232464335142	1.83595157411489	1.34706358791853
Si	3.27332892774349	-0.02099915279117	-4.30223952466226
C	2.32297944490581	3.61767538326298	-3.67688244885750
P	2.14907405426580	5.17516035016528	1.60427381586702
Si	0.58468796535709	0.33623499124453	-2.42737104732581
C	2.02692675246255	4.77030308009640	-4.44532741810765
P	5.48102580111600	4.68395825085633	0.60172918716805
Si	1.25895997534560	7.20485798431839	-3.26536560170412

C	1.17825830431008	4.65042571025622	-5.56837353936606
H	0.96868770533071	5.55418688757085	-6.15594968816330
Si	3.71933199981608	6.87717704634298	-5.43864362783182
C	0.63290664050382	3.41460803289598	-5.95497427210964
C	0.94066822883586	2.28501647066061	-5.17090352610570
H	0.54638182774875	1.30066110334801	-5.46155557601814
C	1.77229780756904	2.36172392261569	-4.03520416710666
C	2.11613613491001	1.10774613110789	-3.26595250092345
H	2.75297310414105	1.39824992808477	-2.39316952297125
C	2.59880262615415	6.11704883550785	-4.08000563940290
H	3.31466986645863	5.98088904790212	-3.23098408383877
C	-0.25231038677730	3.25369883382832	-7.20298580942154
C	0.44328260258475	2.28149676455127	-8.18617210652288
H	-0.17055146542526	2.14281220066079	-9.10092577626336
H	0.60202731881406	1.28392203051455	-7.72992711442819
H	1.43543028298589	2.67293122963543	-8.49038337886127
C	-1.62445027900012	2.67477507531122	-6.78428002285460
H	-2.28246866377514	2.54744053831459	-7.66937100126263
H	-2.13515867600074	3.34995906466229	-6.06763174996199
H	-1.51950450478382	1.68434238006165	-6.29802238313949
C	-0.48612701066654	4.59436630361236	-7.92413291193099
H	-1.12991324163821	4.43878498025690	-8.81371668872275
H	0.46509137174345	5.04437750754487	-8.27369580581616
H	-0.99270427837744	5.33114594782182	-7.26806541018236
C	4.21392657939418	1.04997052730110	-5.53922820369212
H	4.94622969792171	0.44263096917074	-6.11106673655358
H	4.76251899504347	1.85924479552205	-5.01419244961491
H	3.51976936193335	1.53118483000648	-6.25736853266318
C	4.50913093219512	-0.84718852022568	-3.12538433729286
H	5.18994992055343	-1.52401864699257	-3.68260817831927
H	4.00472052226401	-1.44480732517536	-2.33934166111318
H	5.13307542453546	-0.07580498348644	-2.62861229924332
C	2.32334391818879	-1.36392526654950	-5.24904642423285
H	3.02888982680395	-1.95817977490586	-5.86688348034492
H	1.57317607827797	-0.91923735378794	-5.93494514659288
H	1.79612814866756	-2.06558505973144	-4.57089643102041
C	-0.72648901712703	-0.31138903063363	-3.63593225705722
H	-1.53068963419637	-0.81764154745310	-3.06093744004055
H	-0.32238408557079	-1.03847718605298	-4.36652638926606
H	-1.19409075508347	0.52259909750434	-4.19664178683317
C	1.14600058328430	-1.11450646063506	-1.33832196924999
H	0.29595110521656	-1.50954755769842	-0.74387831223722
H	1.94432729339084	-0.81777502748430	-0.62955943027967
H	1.53889602239838	-1.94797918317583	-1.95652711945057
C	-0.24581220788019	1.67945253738477	-1.38523321272466

H	-1.10090970004340	1.27873984705948	-0.80217792008926
H	-0.62576675169315	2.48167936981707	-2.05125196776657
H	0.47409209710129	2.15816277036482	-0.68910700638148
C	0.42495137334524	6.14457072974820	-1.94073276863823
H	-0.26546267726585	6.74416573128038	-1.31206193369665
H	1.19384516851036	5.67033999344700	-1.29529743132206
H	-0.15332714921736	5.32361752944543	-2.41160939592343
C	2.11719819044079	8.69073601678867	-2.45538989544926
H	1.40612984939080	9.28213717567448	-1.84177213631106
H	2.55627323767308	9.37190475454319	-3.21305115128895
H	2.93975837989763	8.34845369380227	-1.79313903436869
C	-0.08389688399327	7.79608028685397	-4.46297653202822
H	-0.85790482724194	8.36198016535438	-3.90268399143481
H	-0.58460787362684	6.92884561883012	-4.93981364315843
H	0.30789519459193	8.45270224080297	-5.26339508624353
C	4.34450890159609	5.50479077256276	-6.57624828927143
H	5.08306976688696	5.90238598225460	-7.30335719063984
H	3.51154823181192	5.04057364005640	-7.14147709549859
H	4.83122618917695	4.70989982800487	-5.97595716381539
C	5.17415901283921	7.70942390351327	-4.55631057916290
H	5.85655099839598	8.20226025679304	-5.27960857406525
H	5.75500782658311	6.94491227486215	-4.00001553883061
H	4.82854872220585	8.47671421804290	-3.83383112346964
C	2.81679539171296	8.17150005268930	-6.49633863628281
H	3.49865946006840	8.54745986567157	-7.28804915281126
H	2.48489506114920	9.04453937111415	-5.89787348120499
H	1.92579372895571	7.74235494812666	-6.99918567934287
C	4.37141081051295	0.46664433583866	0.40190944737227
H	4.41413285089221	-0.48645966540489	0.97026577303781
H	5.39459176875376	0.78470155778062	0.12429017878137
H	3.80968504038528	0.31737773980769	-0.53829403596860
C	1.97916255876162	1.04067812417770	1.88256040927144
H	2.14385086648773	0.05035954476444	2.35496331084361
H	1.32392299170762	0.92560612162933	0.99866867096010
H	1.46689686002428	1.70974898352410	2.60185202798839
C	4.53110047025418	1.77286548915568	2.93054402171882
H	4.52355629425496	0.75755861741228	3.37906205414489
H	4.10460147952583	2.49530965485890	3.65294462784935
H	5.58031774390022	2.06386949172403	2.72733852204815
C	0.31962891132772	4.91487188517889	1.53761377749416
H	-0.22213266209798	5.59720899761458	2.22457067798089
H	0.10689236219654	3.86340720520153	1.81147260116046
H	-0.02676052829054	5.07267955708528	0.49966837471235
C	2.41522305166055	5.04662501269066	3.44076436505146
H	1.77418156338021	5.75573592513616	4.00519596520009

H	3.47620713852558	5.24054130288991	3.68508091107645
H	2.17263529575038	4.01293004114016	3.75749420651722
C	2.28349084146489	7.00949596571978	1.36323374439662
H	1.62040005208489	7.57756721922160	2.04899003101786
H	2.02373866108622	7.24440836995163	0.31358082028303
H	3.33320193671848	7.32043549809354	1.53317674550308
C	6.91264428160987	3.58956285805413	0.19218528169823
H	7.88566007552187	4.09787617609895	0.35126223311092
H	6.81511145507419	3.29605116364044	-0.87209883805498
H	6.86811573557062	2.67842710403700	0.82060452365134
C	5.91898578070542	5.22891796829865	2.32177122608516
H	6.97361066868074	5.56726832354144	2.38052596651772
H	5.76201822889684	4.39757157157272	3.03472458914682
H	5.26068644463217	6.06967938651041	2.61622434212480
C	5.88598196821560	6.21653833801535	-0.34812844585219
H	6.88641362847369	6.61704915965016	-0.08453757385706
H	5.10925365494216	6.97868556439552	-0.14545938864118
H	5.85875867213619	5.96651803358977	-1.42690972278214
H	1.86881136262938	3.27261141980408	-0.25530560329218

Compound 3



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Coordinates from ORCA-job optfreq_wB97X_hnumac

C	1.44789892558909	3.61493361214963	-3.74477748030182
C	0.62220900380862	6.12688414513987	-2.68075944017982
C	2.95711426377621	4.90441895694234	-1.74599532473794
C	-2.17524968140498	-2.52920008681932	-2.89293898106599
C	-4.51116423244255	-0.57921236039171	-2.75904798655127
C	2.15106288408326	-0.47093170586348	-2.98761046404425
C	-4.58955966170760	-3.17343194134991	-1.12496513029572
C	3.22801520100947	-3.17922560001388	-2.10656583922710
C	5.02017715567519	-0.69631900872691	-1.91963700844827
C	-0.99308745015531	-5.82433927935603	0.00061632201588
C	-2.19140061843222	6.12864743509433	-0.71435996800641
C	-2.58256838070095	-0.83865654489066	-0.34494135127883
C	2.82847821330536	3.52070637825767	1.37905122161022
C	-1.26996141085724	-1.49832918421821	-0.00403055808560
C	-1.29083124513658	-2.83462101518432	0.39059101117386
C	1.10308875751069	5.75086220944724	1.60683773259695

C	-0.01373555712051	-0.83652645233801	-0.09812362806953
C	-0.12379199779337	-3.56899707846874	0.63000819731356
C	-0.24915597497744	-5.02564943827311	1.08805796155454
C	1.18488784124793	-1.56190134603929	0.12786130480757
C	-5.27035602088254	0.23916641381572	0.80429325452208
C	1.09984553901615	-2.92248324671962	0.45892648197470
C	-3.54118144215187	3.66247093079290	-0.94711001743179
C	2.55652827409275	-0.94281792959072	0.01185153920234
C	1.11652346272841	-5.67760796094325	1.34620203413627
C	-1.04422834396708	-5.03838152891750	2.40872272819156
C	-3.83247503151808	-2.00972026203340	2.33521994199215
C	-2.58767102161617	4.55839965108857	1.57295668557524
C	4.69345773984596	-2.94928631507452	1.24089267864950
C	0.48438738275526	3.27158122114043	2.89141623642049
C	-2.55483493231360	0.72459015682423	2.22192270271399
C	4.88042595645311	0.07868946045972	1.73437037468861
C	2.69278017301731	-1.58419080016947	3.07119959468762
Si	-3.47489940870307	-1.78786587520048	-1.75359306620368
Si	3.25590169646767	-1.33619819808741	-1.73039921724407
Si	-3.58966602381589	-0.50132805904573	1.23780952937822
Si	3.69978820090948	-1.36758953570547	1.48815657121920
P	1.21492908340180	4.47275889159175	-2.14174785208851
P	-2.04208056995056	4.38105524649829	-0.17403122627476
P	1.05085910635452	3.94569133715320	1.28619764946545
Ge	0.06008743363620	1.06698238667783	-0.35218969050971
Ir	-0.07605965468981	3.25368399922613	-0.62900522739371
H	1.99790963450824	4.24944544164518	-4.45633484245138
H	1.31281435842922	6.56323234142423	-3.41792432694386
H	-2.67202060797680	-3.08886919340292	-3.70314568325270
H	3.41782220769396	5.42922405476104	-2.59721253903211
H	0.46839218532021	3.34851548614558	-4.16543780667071
H	-5.09223986642552	-1.13693322814046	-3.51225367736038
H	3.52809902913482	3.98925316237978	-1.53667720722726
H	2.01132750512950	2.68577119322742	-3.57955006973564
H	2.55706104699881	-0.60955318506089	-4.00366443566098
H	-5.07445323020432	-3.65882710481797	-1.98893788321361
H	0.55525380606119	6.80087911870325	-1.81475645643275
H	-1.55242245383649	-1.74444612640455	-3.35496559528948

H	-0.37211189602657	6.05094159364983	-3.14207582264665
H	-3.86231447524652	0.13158721543545	-3.29802462169408
H	-1.50829805920655	-3.22067694988547	-2.35562201977384
H	1.13177227949479	-0.88878509686124	-2.97291560730707
H	3.00860904858217	5.56520303658300	-0.86967425839614
H	3.80236623294547	-3.36404081565165	-3.02953147988899
H	-5.22179408585399	-0.00237295456341	-2.14808706860273
H	2.07480783773278	0.61246936128245	-2.79959544444807
H	-4.04099873355722	-3.95812988464186	-0.58147296387073
H	5.41648000459214	-1.02830549506552	-2.89318417610979
H	2.20249187226000	-3.54770590630873	-2.26277144569998
H	-5.39072431331958	-2.80023948880582	-0.46819488975413
H	-0.37462917661619	-5.91201320575224	-0.90673722624173
H	-2.08677776553224	6.20062802145947	-1.80464032653301
H	-0.86835255052484	2.83727581259176	-1.99504189509979
H	3.40329132607836	4.12526360407048	0.67101340454486
H	-1.93951312188307	-5.34177929687221	-0.28584266386321
H	-1.40798955249233	6.73832482710075	-0.24319836608078
H	3.69232933983649	-3.78254485403063	-1.31401236720338
H	-1.22892165295721	-6.84011354866966	0.35610069332578
H	1.46893221174812	6.26958766672062	0.70942241623142
H	5.07865337142669	0.40448096360300	-1.89812340437324
H	-2.40395732450815	0.17140374822128	-0.76838589193895
H	5.69677419724528	-1.08864715810825	-1.14555666528624
H	-3.46247830886218	3.73369443878533	-2.04134374305441
H	-3.17491419547041	6.53089329978605	-0.42686431718127
H	-5.91982097514199	-0.51013546660488	0.32535969173612
H	1.70925349984192	-5.75688257730070	0.42141569357356
H	-2.25722099062351	-3.32544891975110	0.49695335430600
H	-5.20226148124232	1.10475090339424	0.12743219372808
H	2.97105970841976	2.46260844434572	1.12015494219239
H	3.21270931998636	3.71166085211187	2.39268281343891
H	0.09827852803705	6.13176913317076	1.83746861678196
H	2.48518014971479	0.16422162155828	0.01926484614371
H	2.02579567053172	-3.47286026181478	0.61628817714583
H	0.97713507577372	-6.69495054257942	1.74448990716828
H	1.77472679148634	5.98646275723151	2.44558972574470
H	-4.44290174611958	4.19954517810228	-0.61548275813756

H	-4.29200727406133	-2.86630852138863	1.82081056035269
H	-5.77837365451796	0.58077405047548	1.72180673181994
H	-3.62791587904931	2.60229030715776	-0.66894040150957
H	-2.06558538690116	-4.64797870975032	2.28392528703786
H	1.69898290829908	-5.11676627896660	2.09234297370563
H	-1.11789423952321	-6.06485535541703	2.80056975627388
H	5.23150878512786	-2.98139183793093	0.28119933472683
H	-2.87790837009549	-2.33825500210703	2.77295907809269
H	5.35078761602790	0.42407015440987	0.80017332484232
H	-1.83913717777731	5.11863167324447	2.14919469783937
H	4.06578844387808	-3.85164131652116	1.31649676249819
H	-3.53679140388209	5.11439133319785	1.62111157035223
H	-4.49783065768816	-1.73612370207616	3.17042513193421
H	-2.28604001557655	1.58929803500317	1.59501529354095
H	-0.53989987916265	-4.41780259269100	3.16674145300678
H	1.01725335713799	3.75747183183437	3.72369019171930
H	0.69922145454331	2.19142551853551	2.91032091248130
H	4.34527641556372	0.92923597310502	2.18749313335922
H	-2.72795249058464	3.57343037792220	2.03675275013323
H	-0.59623380355154	3.40812255083242	3.01902414871094
H	-1.61716561936903	0.24112358418656	2.54668837815883
H	5.45047826902703	-3.01184916522310	2.03890776266574
H	1.89553285104117	-2.33324855409067	2.95988916537166
H	-3.07887561879020	1.08345309299758	3.12245948053279
H	2.21807724254308	-0.64499762045415	3.40245519481207
H	5.68751923852039	-0.20387852570864	2.42913853146754
H	3.36694757909189	-1.92794499585179	3.87437997001722

Compound 4

XYZ-files

4-BP86

C	-0.212112864	1.069268505	-3.008917128
C	-1.036134064	3.759017034	-3.650649411
C	1.740627122	3.155068799	-3.365915051
C	-2.244599863	-1.815454680	-3.377886976
C	-4.168423396	0.549857122	-2.744454469
C	3.273388326	-0.124198348	-2.124621074
C	-4.758897443	-2.317062646	-1.772085993
C	4.387422267	-2.776460237	-1.009052483
C	5.485708876	-0.069721426	0.025942553
C	-0.615142967	-5.426467184	-1.670385574

C	-1.817534468	6.252154980	1.060488981
C	-2.418080313	-0.553635544	-0.483318140
C	3.168874493	3.689372294	-0.112088130
C	-1.135895195	-1.320968053	-0.262677730
C	-1.154797147	-2.726048015	-0.364120636
C	1.850262061	6.173983570	-0.831626131
C	0.084748265	-0.671951166	0.088802832
C	-0.010539427	-3.519466954	-0.148613336
C	-0.114608055	-5.049273240	-0.255347512
C	1.254916597	-1.457993612	0.294613055
C	-5.097257494	0.365592825	0.855460453
C	1.190738957	-2.862282852	0.169869063
C	-3.523647030	3.940311783	1.139670773
C	2.560734490	-0.824204539	0.727305860
C	1.239907378	-5.740472057	-0.011981439
C	-1.124863943	-5.552855768	0.804134481
C	-3.818978464	-2.344667761	1.713434081
C	-1.411961037	4.195300339	3.064296265
C	4.034693270	-2.798057228	2.708572916
C	1.856103312	5.211686103	1.874831678
C	-2.485977077	0.288798573	2.472525555
C	3.888318486	0.256937371	3.293817564
C	1.347768418	-1.467718802	3.487787303
Si	-3.386594552	-1.044889442	-2.075344350
Si	3.948500329	-0.990713782	-0.582160063
Si	-3.481325026	-0.590153248	1.109699155
Si	2.982110949	-1.236439195	2.560461654
P	0.114661801	2.813122790	-2.557936557
P	-1.750930436	4.416939189	1.264935322
P	1.593701611	4.624023556	0.142517661
Sn	0.255508632	1.341487708	0.995714008
Ir	-0.403600809	3.446042292	-0.391820818
H	0.051177177	0.868226795	-4.065784920
H	-0.885636906	3.480278641	-4.713517383
H	-2.782866980	-1.877631531	-4.346908059
H	1.665003261	2.969902321	-4.456133462
H	-1.288611711	0.882318116	-2.851793836
H	-4.722716894	0.354489271	-3.685438576
H	2.519698477	2.486610334	-2.954876088
H	0.345551565	0.390568984	-2.335568374
H	4.033131404	-0.032330589	-2.927330596
H	-5.270297119	-2.531281904	-2.733771365
H	-0.858058160	4.845378072	-3.530203186
H	-1.309796687	-1.247531795	-3.539543285
H	-2.078703306	3.539332618	-3.352287645
H	-3.404760400	1.326332719	-2.958120298
H	-1.954342423	-2.844409151	-3.087707163
H	2.400985237	-0.673882166	-2.531669369
H	2.039972991	4.207796655	-3.203196316
H	5.243492730	-2.785106948	-1.715723679
H	-4.882781014	0.980457073	-2.014395516
H	2.932942200	0.895234258	-1.849982394
H	-4.350091760	-3.278101596	-1.398296739
H	6.253628441	-0.036062944	-0.774557773
H	3.538933772	-3.292090021	-1.500709114
H	-5.530530650	-1.973253117	-1.055562766
H	0.079604006	-5.053946463	-2.450351399
H	-2.103635824	6.488421935	0.017118027
H	-1.775003349	2.658581753	-0.829672256
H	3.224100075	3.299626874	-1.143607606

H	-1.618257832	-5.003172905	-1.878720967
H	-0.821659374	6.693140491	1.257451031
H	4.680895119	-3.363701240	-0.116817388
H	-0.690621683	-6.528303460	-1.773859677
H	1.855737414	5.938778462	-1.913252596
H	5.251565287	0.976775747	0.311307216
H	-2.179357917	0.527084467	-0.619962961
H	5.944598421	-0.567122351	0.904406240
H	-3.877268776	4.143479424	0.110953640
H	-2.556251458	6.705177648	1.752003054
H	-5.797851343	-0.179023790	0.191936992
H	2.003587892	-5.425399149	-0.751633142
H	-2.106974550	-3.219434991	-0.609907206
H	-4.918601816	1.361344901	0.401831745
H	3.180090412	2.827639824	0.585677649
H	4.054718925	4.325204810	0.087538761
H	1.007249731	6.866044537	-0.639382745
H	2.456529357	0.295928366	0.734445513
H	2.101118189	-3.446600153	0.350673728
H	1.124480233	-6.839149889	-0.100217051
H	2.802022928	6.675333992	-0.563987831
H	-4.146790717	4.495593336	1.868926152
H	-4.397827311	-2.938456020	0.979820774
H	-5.612069770	0.520325476	1.826240622
H	-3.619816498	2.854426699	1.325664343
H	-2.132962647	-5.118726309	0.650410339
H	1.634449958	-5.529339873	1.002706894
H	-1.222545304	-6.656764246	0.753640395
H	5.019650554	-2.681003485	2.212817949
H	-2.868412052	-2.878023351	1.914872200
H	4.859729322	0.447889988	2.796746860
H	-0.385812271	4.526542484	3.303819740
H	3.525016823	-3.674676631	2.259317171
H	-2.138267360	4.767307026	3.675982050
H	-4.400644989	-2.314060061	2.658099384
H	-2.212696378	1.321599164	2.160291084
H	-0.792429775	-5.283594669	1.827476445
H	2.844983608	5.700310424	1.983712104
H	1.805246585	4.340455192	2.557428364
H	3.264835397	1.171479653	3.195936874
H	-1.492039334	3.119340991	3.314638148
H	1.069797978	5.935274577	2.162278316
H	-1.558498593	-0.273849027	2.709830229
H	4.223158317	-3.032438275	3.776699749
H	0.727739782	-2.258739921	3.019835591
H	-3.062975986	0.385142544	3.415713506
H	0.758365001	-0.525557143	3.482331614
H	4.086035301	0.103861256	4.374987273
H	1.526308480	-1.741861786	4.547764749

4-M062X

C	0.985817786	3.610541559	-4.062552976
C	0.133584151	6.195021367	-3.135675381
C	2.635952456	5.131988961	-2.392649915
C	-2.116659273	-2.317520175	-2.916708640
C	-4.464877235	-0.396991995	-2.630388306
C	2.621760374	-0.472296693	-2.672416449
C	-4.526058096	-3.031881065	-1.115076688
C	3.341077025	-3.328916109	-1.859680664

C	5.329247396	-1.023918540	-1.398423883
C	-0.035623685	-5.837134854	-0.556057156
C	-2.720660387	5.934165918	-0.955898452
C	-2.458536299	-0.772785009	-0.263427899
C	2.938365191	4.033269859	1.002134326
C	-1.173918580	-1.498890251	0.057085628
C	-1.295638360	-2.853071307	0.374021860
C	1.257757076	6.296310603	1.081150954
C	0.116245310	-0.921784832	0.046746321
C	-0.194752528	-3.671885231	0.585750009
C	-0.385324846	-5.170192818	0.787497800
C	1.265304732	-1.717535751	0.311763895
C	-5.145720292	0.251061001	0.996788704
C	1.076800254	-3.086726688	0.535603401
C	-3.682446984	3.345439757	-0.143123965
C	2.684229137	-1.179525427	0.332047887
C	0.515923282	-5.667117665	1.926696536
C	-1.838147999	-5.515062360	1.147866357
C	-3.681714670	-2.042570914	2.386868871
C	-2.445389573	5.014338135	1.706698898
C	4.610502272	-3.414376168	1.567633579
C	0.754615555	4.033617521	2.735438400
C	-2.334825243	0.657960986	2.393504904
C	5.040879907	-0.442607564	2.227832675
C	2.660524130	-1.990088829	3.372120613
Si	-3.395472471	-1.643365927	-1.710078503
Si	3.507952543	-1.515797587	-1.377673489
Si	-3.439039468	-0.480560169	1.363154995
Si	3.740409100	-1.759498614	1.848359311
P	0.866573213	4.618840212	-2.527987771
P	-2.207793447	4.433164439	-0.026064342
P	1.149413441	4.463244973	0.992412942
Sn	0.225739536	1.185531769	-0.331259471
Ir	-0.213177107	3.577058395	-0.733342858
H	1.445298297	4.191047879	-4.875799128
H	0.717713307	6.593509143	-3.978227956
H	-2.621441997	-2.891697457	-3.709554390
H	2.963437216	5.612811877	-3.326529087
H	-0.006984830	3.254473460	-4.368606390
H	-5.039357809	-0.932395600	-3.402312894
H	3.256462745	4.243945609	-2.213004188
H	1.612936648	2.734401315	-3.848188433
H	3.041617686	-0.692291528	-3.667194230
H	-5.037676324	-3.466903941	-1.988370076
H	0.136981220	6.929197856	-2.318065597
H	-1.552777936	-1.501535156	-3.397426751
H	-0.903359257	6.038837588	-3.461336438
H	-3.843074717	0.356731084	-3.139157677
H	-1.396271633	-2.979472911	-2.414018147
H	1.546333685	-0.712651940	-2.708091062
H	2.787676546	5.842819737	-1.570147707
H	3.961705250	-3.530279332	-2.746158050
H	-5.183385553	0.120781283	-1.978700958
H	2.747813510	0.608640092	-2.492397857
H	-4.003823764	-3.853709778	-0.606686516
H	5.773674704	-1.377729241	-2.341126361
H	2.300176383	-3.591844353	-2.098556111
H	-5.305804389	-2.652109223	-0.437249235
H	1.026014720	-5.691724847	-0.809130200
H	-2.782535377	5.689071232	-2.025050947

H	-1.169244392	3.058078346	-1.933942647
H	3.388784834	4.276140617	0.033122166
H	-0.637851944	-5.390932523	-1.361560154
H	-1.956760102	6.712434572	-0.821838132
H	3.687374114	-4.002090565	-1.063217698
H	-0.248032522	-6.917117494	-0.529221215
H	1.623379863	6.691366612	0.123208037
H	5.469204928	0.067043812	-1.355910966
H	-2.265043114	0.251413932	-0.652252155
H	5.907209642	-1.478431041	-0.581989983
H	-3.798543855	2.945928891	-1.160407187
H	-3.691266205	6.314507664	-0.605455516
H	-5.821594859	-0.547474121	0.655712669
H	1.585692305	-5.556756958	1.696041057
H	-2.294344633	-3.276737206	0.420463961
H	-5.144170669	1.035346006	0.228383034
H	3.060176873	2.957798023	1.196827614
H	3.458287783	4.598873939	1.786566907
H	0.266827200	6.727500090	1.277789496
H	2.678412322	-0.071953870	0.420034638
H	1.960270096	-3.708578434	0.685834510
H	0.331122442	-6.732813942	2.125382492
H	1.949401252	6.609548172	1.874593273
H	-4.592631066	3.882623131	0.162639778
H	-4.156934115	-2.860212727	1.826692445
H	-5.580017619	0.682370436	1.913170473
H	-3.525040364	2.505388675	0.545729632
H	-2.517314865	-5.365155469	0.296401399
H	0.304675396	-5.104180006	2.848984789
H	-1.904314075	-6.573248464	1.438102076
H	5.177229077	-3.472154740	0.627401753
H	-2.726684536	-2.405795364	2.792810822
H	5.569025385	-0.080254871	1.333468382
H	-1.678458101	5.746218037	1.991785403
H	3.907005592	-4.260503126	1.604005432
H	-3.430245744	5.495026492	1.798459187
H	-4.337150703	-1.803992093	3.238700767
H	-1.980778311	1.531375976	1.819666855
H	-2.201652928	-4.913922931	1.994758738
H	1.408178571	4.591486689	3.419907861
H	0.923959231	2.956468634	2.878607839
H	4.587912388	0.423759735	2.734065761
H	-2.401514873	4.155558236	2.389514481
H	-0.289545099	4.262708249	2.971847864
H	-1.452383376	0.079756184	2.716489369
H	5.329801558	-3.560804216	2.387662775
H	1.885751173	-2.751462882	3.206507195
H	-2.845242221	1.025117276	3.297138987
H	2.161779187	-1.061277371	3.689020874
H	5.793724411	-0.861793683	2.912280102
H	3.301789015	-2.335350087	4.199169091

4-M062X

C	2.809074166	3.920137825	-2.859362163
C	0.318486264	4.917604397	-3.806751845
C	1.781234546	6.394053318	-1.914122369
C	-2.360802131	-2.193942220	-2.588899140
C	-4.477853822	-0.072305433	-2.174471483
C	2.277723596	-0.731138989	-2.758690855

C	-4.697744195	-2.665207733	-0.618036453
C	3.098335888	-3.565655436	-2.049573742
C	5.146826170	-1.309977609	-1.834668180
C	-0.998312133	-5.633956179	-0.710357932
C	-2.255704859	5.965850508	-1.240972344
C	-2.354416418	-0.609701490	0.039044391
C	2.600403369	4.645267723	1.497159972
C	-1.105273453	-1.437622751	0.248116287
C	-1.276764386	-2.800164641	0.490123166
C	0.346049670	6.353500957	1.409038065
C	0.215810691	-0.917892208	0.172041772
C	-0.203013433	-3.689410703	0.577750581
C	-0.470193139	-5.191207268	0.669723232
C	1.321770433	-1.794221078	0.312354153
C	-4.765711947	0.757404836	1.423970903
C	1.082187627	-3.163101876	0.490244650
C	-3.263161029	3.323781359	-1.575843456
C	2.768012255	-1.369611523	0.202093024
C	0.806595528	-5.974300564	1.010735613
C	-1.520830728	-5.463181615	1.758338602
C	-3.520414446	-1.748275006	2.739326635
C	-2.923161505	4.409659690	1.018421366
C	4.585297536	-3.798425169	1.212522524
C	0.228559682	3.953871443	2.883435674
C	-1.932525896	0.852994861	2.654524675
C	5.289084005	-0.888005822	1.899160064
C	2.876746628	-2.299108878	3.188895534
Si	-3.474613773	-1.399907343	-1.298313562
Si	3.338428145	-1.756586930	-1.584098355
Si	-3.173034107	-0.211983287	1.712256085
Si	3.871138829	-2.093259056	1.599052970
P	1.247766827	4.666161118	-2.245807019
P	-2.044425468	4.260433057	-0.586021577
P	0.786323614	4.579569212	1.252515250
Sn	0.489620460	1.158832933	-0.083821698
Ir	0.084178248	3.447567052	-0.646408893
H	3.265573315	4.541335352	-3.645310347
H	0.939950055	5.414181103	-4.567326242
H	-2.971104813	-2.704075353	-3.352843435
H	2.338421781	6.798429674	-2.773198375
H	2.598128404	2.921417902	-3.270149989
H	-5.158027502	-0.567299779	-2.887351937
H	2.424754117	6.446873080	-1.025102283
H	3.516651228	3.808208441	-2.025741052
H	2.593266562	-0.920354147	-3.798564048
H	-5.281578821	-3.079084674	-1.457577450
H	-0.558426293	5.547035883	-3.606753955
H	-1.750730019	-1.427484109	-3.097646300
H	-0.034112145	3.948727038	-4.188028975
H	-3.817408619	0.592244086	-2.754188635
H	-1.674596165	-2.929528183	-2.145376379
H	1.216017469	-1.016831519	-2.674794723
H	0.896127764	7.023410606	-1.744559395
H	3.575003073	-3.743923021	-3.028307003
H	-5.093750985	0.540044637	-1.498036244
H	2.368790368	0.354366584	-2.578388995
H	-4.224787754	-3.514976162	-0.102324911
H	5.451768634	-1.615270942	-2.849394264
H	2.033548836	-3.832435223	-2.134747651
H	-5.414893045	-2.196813954	0.075044713

H	-0.243835854	-5.438476187	-1.489563784
H	-2.163089029	5.954867529	-2.335744519
H	-0.414793650	2.616375747	-1.975498913
H	3.085966989	4.984697844	0.571714986
H	-1.911059893	-5.080875726	-0.981587643
H	-1.476155722	6.625053360	-0.835996548
H	3.565932489	-4.254712326	-1.333119340
H	-1.238215421	-6.709894224	-0.721679840
H	0.800181125	6.925491087	0.591068836
H	5.336381479	-0.229026161	-1.737499615
H	-2.095505550	0.383682666	-0.379212006
H	5.803419341	-1.839576866	-1.128845924
H	-2.872154742	3.173043242	-2.591644324
H	-3.244899620	6.371905478	-0.979075919
H	-5.551529446	0.113137831	0.999801166
H	1.536071672	-5.943755545	0.186108673
H	-2.292256518	-3.185257454	0.554206631
H	-4.617127367	1.601295234	0.733274325
H	2.972523098	3.637229321	1.731005091
H	2.869562082	5.332242821	2.313361074
H	-0.741914304	6.492692226	1.368031551
H	2.872833202	-0.269559364	0.297242180
H	1.939686830	-3.829055480	0.546064997
H	0.563758792	-7.031168425	1.201760861
H	0.715373846	6.754726827	2.364268506
H	-4.230022363	3.848386191	-1.623738602
H	-4.099311108	-2.505749172	2.192897568
H	-5.147242510	1.169899620	2.373215580
H	-3.415450226	2.335952000	-1.121268720
H	-2.493601560	-5.007307398	1.517509621
H	1.287146010	-5.577866927	1.919597292
H	-1.681579398	-6.546236199	1.871055079
H	5.117043460	-3.853264270	0.250608461
H	-2.584690334	-2.217292118	3.081513199
H	5.775312367	-0.560666970	0.965973614
H	-2.405663604	5.121130490	1.675144503
H	3.815401854	-4.585990872	1.228340485
H	-3.950731372	4.773177312	0.861208120
H	-4.102794144	-1.471536665	3.633543320
H	-1.618290218	1.720509976	2.052570613
H	-1.183942265	-5.061823958	2.728279071
H	0.719464571	4.513451469	3.695126659
H	0.470504908	2.885755300	2.979818102
H	4.941173011	0.009293503	2.437083095
H	-2.958015012	3.433081583	1.520148680
H	-0.859551201	4.063396536	2.980757938
H	-1.034073117	0.255117645	2.888037724
H	5.315808849	-4.049928029	1.997874436
H	2.049058034	-3.010206945	3.054635333
H	-2.343457051	1.231385792	3.605055131
H	2.445321238	-1.352579922	3.555802562
H	6.058076857	-1.366772934	2.526418445
H	3.539127741	-2.702915294	3.973155945

[MeSn-Ir(H)(PMe₃)₃]⁺-BP86-free

C	0.326907864	2.180304343	-3.781977737
C	-0.007955104	5.061190050	-3.799211483
C	2.552810892	3.873336198	-3.184719977
C	-2.204089411	5.963347478	0.987647440

C	3.266886216	4.249882679	0.324244217
C	1.853126234	6.680686231	-0.403635325
C	-3.462195650	3.437880464	0.413394824
C	-1.660339411	3.635486144	2.639522031
C	1.468349728	5.445649633	2.158875361
P	0.753333701	3.693575341	-2.823273464
P	-1.835587790	4.157521124	0.878252863
P	1.590754087	5.019482935	0.364585276
Sn	0.477022882	1.429921994	0.118801975
Ir	-0.156572638	3.781867792	-0.671288459
H	0.646798210	2.272832774	-4.839056778
H	0.339814266	5.035138662	-4.851556369
H	2.730455406	3.850571090	-4.278724469
H	-0.765778842	2.014898388	-3.732654066
H	3.109089557	3.039533164	-2.713693569
H	0.835845498	1.306040565	-3.328219761
H	0.262792757	6.036655692	-3.350724920
H	-1.109430351	4.956521011	-3.771914412
H	2.936130771	4.830798307	-2.783422551
H	-2.421909305	6.349966105	-0.026801896
H	-1.355852921	2.995866737	-1.453875299
H	3.564656913	4.031220961	-0.716194591
H	-1.330849716	6.510080095	1.391077893
H	2.095558448	6.562629118	-1.477503825
H	-3.744063973	3.808040614	-0.590565184
H	-3.080365343	6.145800659	1.641688596
H	3.226655704	3.289976997	0.876223440
H	4.022224020	4.912795061	0.791423476
H	0.920109108	7.272581568	-0.326211236
H	2.675951469	7.233357445	0.092394440
H	-4.244679651	3.714205982	1.147852376
H	-3.370634497	2.336705485	0.364411466
H	-0.747162982	4.072986520	3.081402092
H	-2.541521958	3.949104060	3.234564595
H	2.342652002	6.045531358	2.481475596
H	1.439995818	4.511212207	2.752639382
H	-1.578786344	2.531287540	2.679926818
H	0.547277936	6.024453822	2.361717999
C	-1.385351905	0.260037766	0.323919499
H	-2.042581923	0.428477033	-0.553927833
H	-1.172770162	-0.824803698	0.413633411
H	-1.939648081	0.568555434	1.236608453

[MeSn-Ir(H)(PMe₃)₃]⁺-BP86-constrained

C	-0.453444000	3.476658000	-3.965436000
C	-0.009404000	6.039456000	-2.747731000
C	2.183699000	4.202622000	-3.096047000
C	-3.363089000	4.578259000	-0.550497000
C	3.246253000	3.427192000	0.549761000
C	2.108138000	6.059155000	0.374970000
C	-2.484919000	3.833153000	2.087508000
C	-1.571755000	6.288127000	0.893393000
C	1.404825000	4.323037000	2.558649000
P	0.422167000	4.254735000	-2.543939000
P	-1.844963000	4.505717000	0.491884000
P	1.634382000	4.309045000	0.727389000
Sn	0.092420000	0.928881000	-0.199797000
Ir	-0.117990000	3.338540000	-0.498632000
H	-0.195511000	3.978085000	-4.919967000

H	0.261310000	6.408471000	-3.757942000
H	2.301820000	4.651273000	-4.103497000
H	-1.545271000	3.538927000	-3.795800000
H	2.518470000	3.147736000	-3.119282000
H	-0.171423000	2.407763000	-4.019568000
H	0.518633000	6.644469000	-1.987006000
H	-1.099600000	6.163520000	-2.598804000
H	2.824442000	4.755901000	-2.382868000
H	-3.711253000	3.546941000	-0.750280000
H	-1.356371000	2.620698000	-1.341428000
H	3.510763000	3.351028000	-0.521515000
H	-3.120224000	5.054178000	-1.520162000
H	2.468879000	6.145709000	-0.667822000
H	-2.838386000	2.798585000	1.914124000
H	-4.169257000	5.152418000	-0.051092000
H	3.129037000	2.400411000	0.947492000
H	4.056940000	3.947620000	1.098686000
H	1.232218000	6.722653000	0.498372000
H	2.914951000	6.393378000	1.057187000
H	-3.315856000	4.449845000	2.487750000
H	-1.662672000	3.793730000	2.826921000
H	-1.259585000	6.829790000	-0.019789000
H	-2.500097000	6.748177000	1.288321000
H	2.304904000	4.710751000	3.076847000
H	1.196560000	3.289609000	2.896420000
H	-0.776339000	6.390758000	1.656063000
H	0.536549000	4.955382000	2.826280000
C	-0.325656000	-1.195643000	-0.429780000
H	-0.275444000	-1.493889000	-1.495667000
H	0.451072000	-1.746004000	0.138918000
H	-1.322852000	-1.443659000	-0.015458000

[MeSn-Ir(H)(PMe₃)₃]⁺-wB97X-D3BJ-free

C	-0.046975941	2.728786450	-3.949491702
C	-0.724676270	5.424653149	-3.334518830
C	1.954075993	4.539346130	-3.140899159
C	-2.233535030	6.281805783	-0.309999396
C	3.304915352	3.751958648	0.012991057
C	1.766052948	6.105649767	0.425246111
C	-3.437945802	3.885239229	0.703816021
C	-1.522154724	5.257434517	2.209561451
C	1.752824649	3.977756603	2.322946686
P	0.253523938	4.019678611	-2.689141540
P	-1.800597168	4.682744588	0.488011655
P	1.626763191	4.282667417	0.521359829
Sn	0.037175235	1.070278877	0.099828787
Ir	-0.222301422	3.341623946	-0.538284816
H	0.181857705	3.111719383	-4.956579350
H	-0.471245769	5.633911953	-4.385429180
H	1.975266554	4.896688862	-4.182467843
H	-1.095813154	2.400217500	-3.907954682
H	2.634366733	3.681793110	-3.044279293
H	0.591490136	1.861968590	-3.729962086
H	-0.525134216	6.321243613	-2.731855985
H	-1.795240347	5.181533802	-3.263413150
H	2.306905000	5.353258988	-2.493888149
H	-2.642018143	6.121073031	-1.316578763
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H	3.488816269	3.975803073	-1.044240015

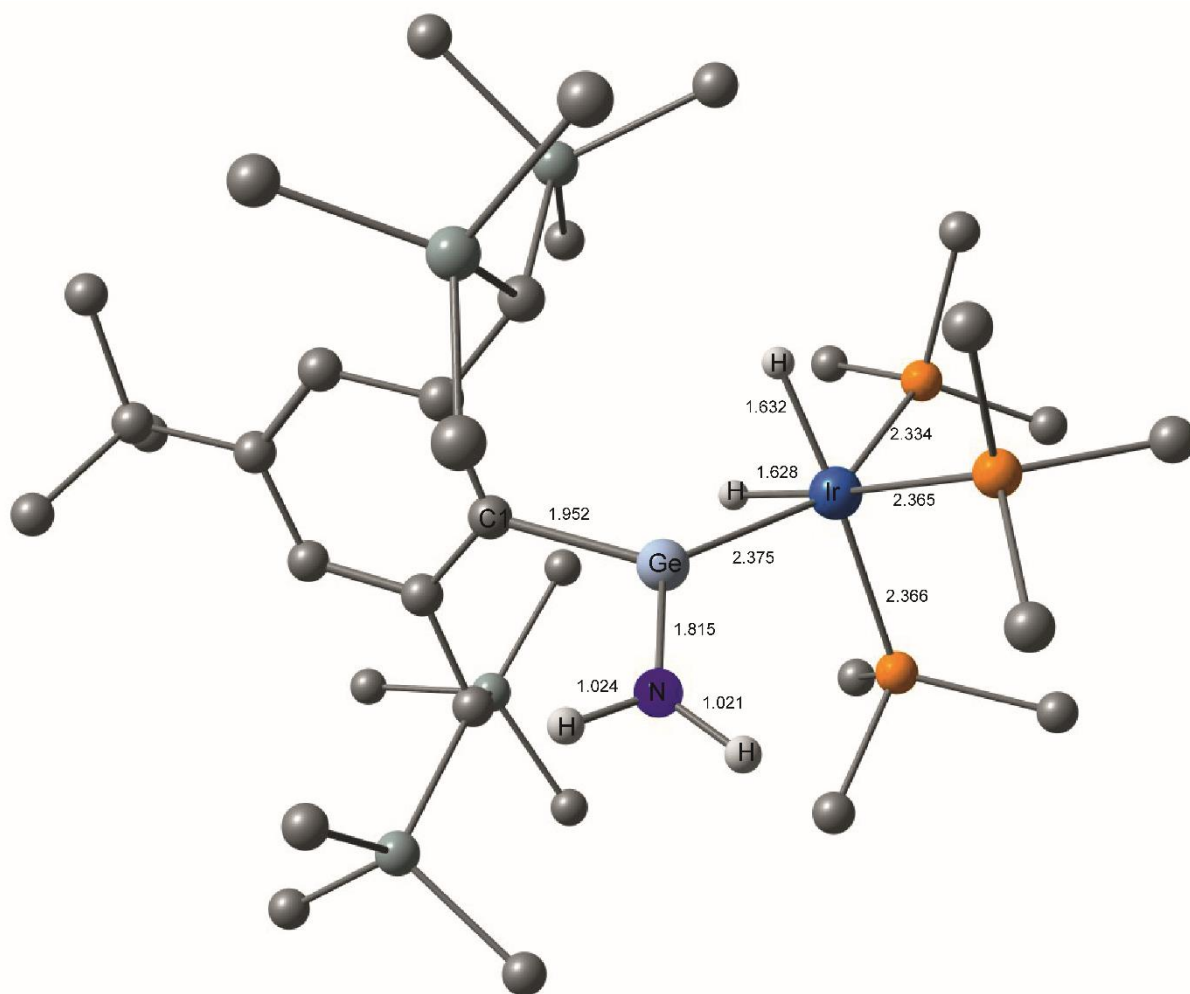
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H	-2.985743877	6.814532656	0.291546821
H	3.396017533	2.665752284	0.162119455
H	4.065017520	4.264822952	0.621199067
H	0.835978792	6.570631362	0.778233113
H	2.599853533	6.473188578	1.039996443
H	-4.150470888	4.580975088	1.174247168
H	-3.316281157	3.004781750	1.350312192
H	-0.594239743	5.837332072	2.303414996
H	-2.358604226	5.899419318	2.524827898
H	2.560233490	4.578803871	2.765583020
H	1.975134054	2.912198451	2.484454102
H	-1.471993400	4.387558156	2.878899947
H	0.809461622	4.214728403	2.825607822
C	-0.023311958	-0.992696813	0.641636898
H	0.256761103	-1.642550345	-0.200770966
H	0.693045714	-1.157777264	1.461295727
H	-1.025723904	-1.266855061	1.007745962

[MeSn-Ir(H)(PMe₃)₃]⁺-wB97X-D3BJ-contr.

C	-0.084899735	2.697625574	-3.900133013
C	-0.650858288	5.420287487	-3.281525908
C	2.001007330	4.449388429	-3.152440977
C	-2.247704479	6.178617944	-0.270278450
C	3.371065216	3.874407544	0.053529379
C	1.781805830	6.223437279	0.338576150
C	-3.372005030	3.731081890	0.717338107
C	-1.533021694	5.197546334	2.253717402
C	1.809965003	4.212223602	2.344819492
P	0.297062533	3.983870061	-2.656838150
P	-1.766421668	4.596980291	0.533873467
P	1.684994321	4.406459115	0.529402088
Sn	0.152916345	1.063137227	0.134981932
Ir	-0.121771681	3.340584079	-0.482726650
H	0.111929627	3.071786007	-4.917139418
H	-0.384303779	5.642577778	-4.326511305
H	2.018850002	4.774467870	-4.204567857
H	-1.138637307	2.394395040	-3.814984106
H	2.664783455	3.581745833	-3.031578809
H	0.541775239	1.816242502	-3.704851092
H	-0.437748622	6.301599377	-2.661203605
H	-1.727282927	5.201590437	-3.224501889
H	2.377122160	5.275667214	-2.534768059
H	-2.626153344	6.007581329	-1.286861126
H	-1.405203657	2.593448047	-1.190960190
H	3.565947582	4.073445957	-1.006776636
H	-1.376906304	6.846619824	-0.329681814
H	1.885493217	6.494181581	-0.721496505
H	-3.731330090	3.378936194	-0.260064730
H	-3.033606824	6.678152161	0.316762788
H	3.464404873	2.792879236	0.231804311
H	4.119767688	4.406621313	0.658943323
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H	2.635601078	6.633736243	0.895886664
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H	-3.228541003	2.855295930	1.365917387
H	-0.680619442	5.886887099	2.321643414

H	-2.433576160	5.739527104	2.582304318
H	2.648724858	4.802961068	2.741021586
H	1.973737280	3.150236972	2.578766852
H	-1.362376672	4.345812587	2.925951320
H	0.886525255	4.536831824	2.834277623
C	-0.329444746	-0.989085268	0.448190018
H	-0.150509338	-1.586763692	-0.458264485
H	0.302490840	-1.391183312	1.254561990
H	-1.382415106	-1.086645658	0.759920141

Compound 5.



Angle C1-Ge-Ir: 128.9°

123

Coordinates from ORCA-job bp86optfreq_hnumac

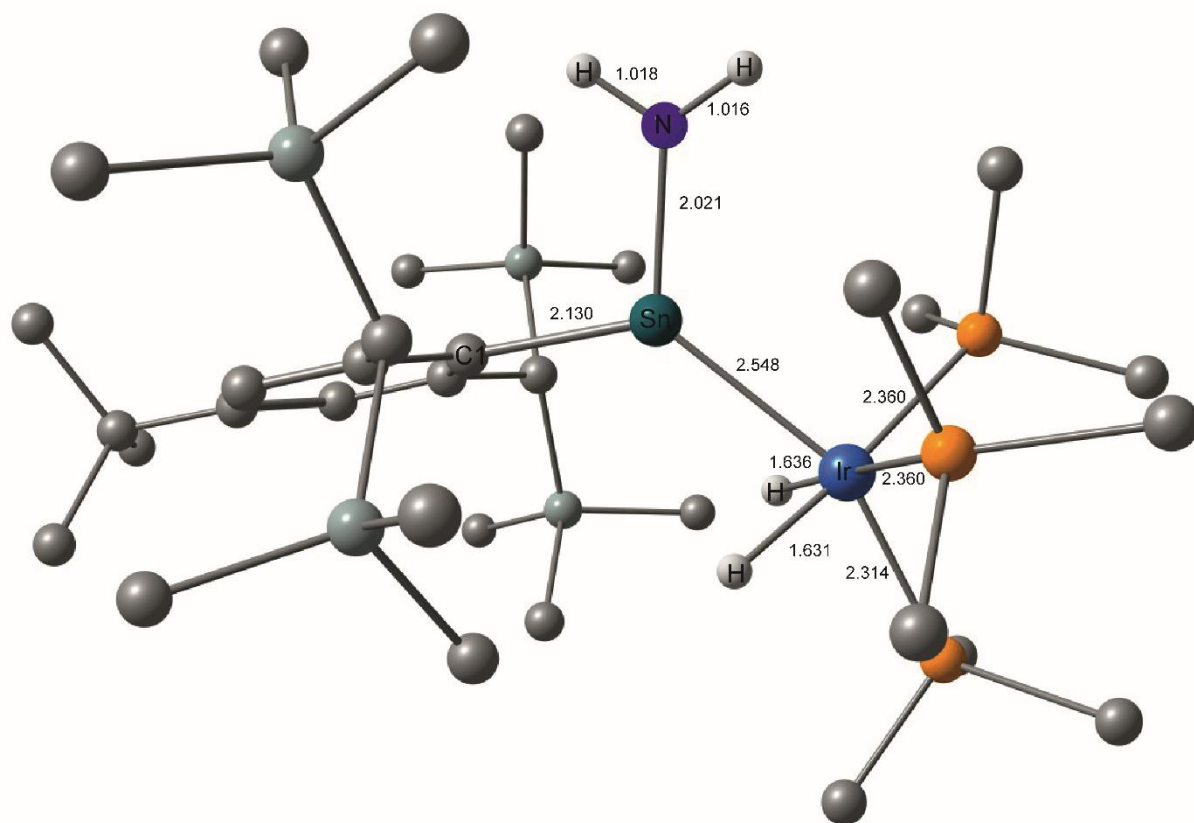
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C	-0.30526450168021	-2.28666161167933	-3.93949569526014
C	-3.60072056175544	2.17780968113984	-2.95587477931164
C	0.32849718337750	3.55096122355167	-2.78947221055860
C	-1.72652718187047	-0.14434429649859	-2.20306240365186
C	-4.88830423865111	-0.39239930700909	-1.80455935337501
C	1.36112392136884	5.73076450083969	-1.26708587702596
C	-2.58303470198139	-5.32789386789047	-1.06457083403858
C	-1.33988908326168	4.82592659490311	-0.85005967949881
C	4.13127333297801	2.86112167648898	-1.18812420716829
C	-1.31319061103712	-1.14888258851491	-1.15786666202985
C	3.26353192446834	-2.69451071010652	-0.72879632846075
C	-2.08260295325396	-2.30534353134299	-0.93316959376316
C	-0.13930758563960	-0.95722852137730	-0.38510539780240
C	-3.19456232788782	1.36691091163639	0.02376189150753

C	-1.73719083789492	-3.25179542648817	0.05391839405225
C	-2.61098024681440	-4.50259615785539	0.24495825267223
C	-4.06309356701967	-4.06792571330211	0.55614439770547
C	0.22874267480377	-1.87720236880334	0.62339240869632
C	4.08005833037518	4.53537696212125	1.13306320899074
C	-0.58726843219176	-3.01234986199717	0.82655403533671
C	2.30587215727591	-4.70066126506332	1.39290428833566
C	-2.10762928553690	-5.39025068247633	1.39854395766489
C	1.44522117956022	-1.64915340145214	1.48429466426121
C	4.32952083957511	1.68143277470548	1.40161377357220
C	4.34813415671421	-2.51198179000932	2.17315111823229
C	0.73083927630069	5.81392461689249	2.38152473203154
C	-1.16083106312907	3.75935175763990	3.07474056940002
C	-0.70931456562782	-0.40144460159724	3.28054341009622
C	1.55387559810097	3.57348147179940	3.97600565047437
C	0.76405810505077	-2.93013327496817	4.30531283073108
C	2.25999205086465	-0.23614678627060	4.11354207612591
N	1.87257608922242	0.29956135087168	-2.18884650704624
Si	-1.50754483968648	-0.82450498085606	-3.99111793310192
Si	-3.37151107837232	0.73228310088312	-1.74999276046146
Si	2.83693820613374	-2.91064758768508	1.10426805278052
Si	0.93942782766491	-1.33252973074417	3.30983684731229
P	0.37598741267784	4.18021845272055	-1.05499136910483
P	3.36079904580789	2.95779306221228	0.49017128378699
P	0.56534444401505	3.97590299410255	2.47508718305298
Ge	0.92491045223374	0.65168448414599	-0.68160630010487
Ir	1.02080412865085	2.63659718343561	0.61829920940851
H	-0.61735600196796	0.26090781617213	-6.08193717160193
H	-2.93025429675741	-1.82741188417689	-5.77521192682688
H	-1.44149669267953	1.46627039130400	-5.04432829707059
H	-3.87203114153628	-0.61011125955405	-4.86162830059420
H	-0.07448080001579	-2.64297867889697	-4.96448478234885
H	0.20603495417369	0.89164094299384	-4.61822326238594
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H	-3.78196780994667	1.81846005876944	-3.98960638497331
H	-0.02701278637175	4.32597982445842	-3.49754081479350
H	0.65363412869027	-2.02913329818779	-3.44493160767658
H	-0.73957786264613	-3.13177638657669	-3.36826592735841
H	-2.71083810537524	2.83967938939834	-2.98396465563775
H	1.33960122072006	3.21842003897005	-3.09178656692878
H	-0.34559515796013	2.67516391613580	-2.84141505005802
H	-4.47232139442442	2.79922357350703	-2.66346934884494
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H	2.44887487991623	0.98469419546709	-2.67960155527587
H	1.78931450366395	-0.59234946186484	-2.68426232345632

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H	-1.00394804906689	0.71181913875531	-2.18473129333197
H	-1.62116599320849	5.51299307862763	-1.67257324748881
H	-2.97433954867755	-4.74683870994673	-1.92377319495826
H	-5.79396008616705	0.21302870804377	-1.59004794682637
H	3.63785801853029	3.57299911252183	-1.87782836285000
H	2.39379731257394	5.47293283214055	-1.57266473797898
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H	3.98865614034725	1.83314230408817	-1.57303927439517
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H	-2.04026419928213	3.96936703247566	-0.82809414087788
H	5.21669582555588	3.08249490004844	-1.15339836996433
H	3.59365486321819	-1.65989034557084	-0.95517050676978
H	1.40887540330530	6.28235122898604	-0.31001197373466
H	-1.42540288441093	5.36158744193826	0.11496802589130
H	-4.50242713761420	-3.47234076811508	-0.26888646061992
H	-2.30693555977060	2.02142697226401	0.14435049168884
H	-4.09572566541320	1.93020243566093	0.34274228615663
H	3.65388775104696	5.39112148743694	0.57562331010994
H	1.50740892427968	-5.00039923106470	0.68526372080199
H	-4.70950183879390	-4.95683389266301	0.70553088743010
H	-3.05707543886276	0.51334592006971	0.71914039245076
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H	-0.55036516045906	2.24112005323777	0.77405899512623
H	-1.07833421622530	-5.76075104516294	1.21813406469653
H	-2.76439136030021	-6.27632269392336	1.50683345854179
H	-4.10441099981235	-3.45343140301951	1.47850491379789
H	1.91867255979344	-0.67638104095915	1.19637913864046
H	5.21370910019669	-3.13240020568063	1.86122544224952
H	0.04708390979300	6.21527088447658	1.60915746371906
H	4.05539540000049	0.68371072830950	1.00588597851594
H	5.42200836421331	1.83380300440309	1.29635883842256
H	-0.30190164077298	-3.72072968137721	1.61282586693380
H	4.64916159524178	-1.44769151447100	2.08635569433109
H	3.82416848697740	4.65356462580507	2.20349384097217
H	1.93827554200872	-4.87378105086014	2.42355400277844
H	1.28148601655857	1.52635781182734	1.78577298163838
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H	4.05313445287621	1.70424098940023	2.47284761222911
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H	0.47711312655896	6.28059290301705	3.35449697806399
H	-1.32103898865369	2.68556394323017	3.29118338707314
H	-0.63669373029219	0.47735870199605	2.60757031883644
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H	2.39040315428899	0.68945231835874	3.51725160404255
H	3.24320142793189	-0.74158645399674	4.18056247046665
H	1.72733604593208	-3.47432574816272	4.38179768693372
H	1.38470414312342	2.51145496848191	4.23437356474741
H	1.26266709689647	4.21556011897400	4.83096462101583
H	-0.99435643590978	-0.05519863933236	4.29570409824531
H	0.42848104544216	-2.69771587863481	5.33747975004262
H	1.95633411423885	0.05340160683305	5.14101908972789

[TbbSn(NH₃)IrH₂(PMe₃)₃]⁺.



Angle C1-Sn-Ir: 130.6°.

123

Coordinates from ORCA-job bp86optfreq_hnumac

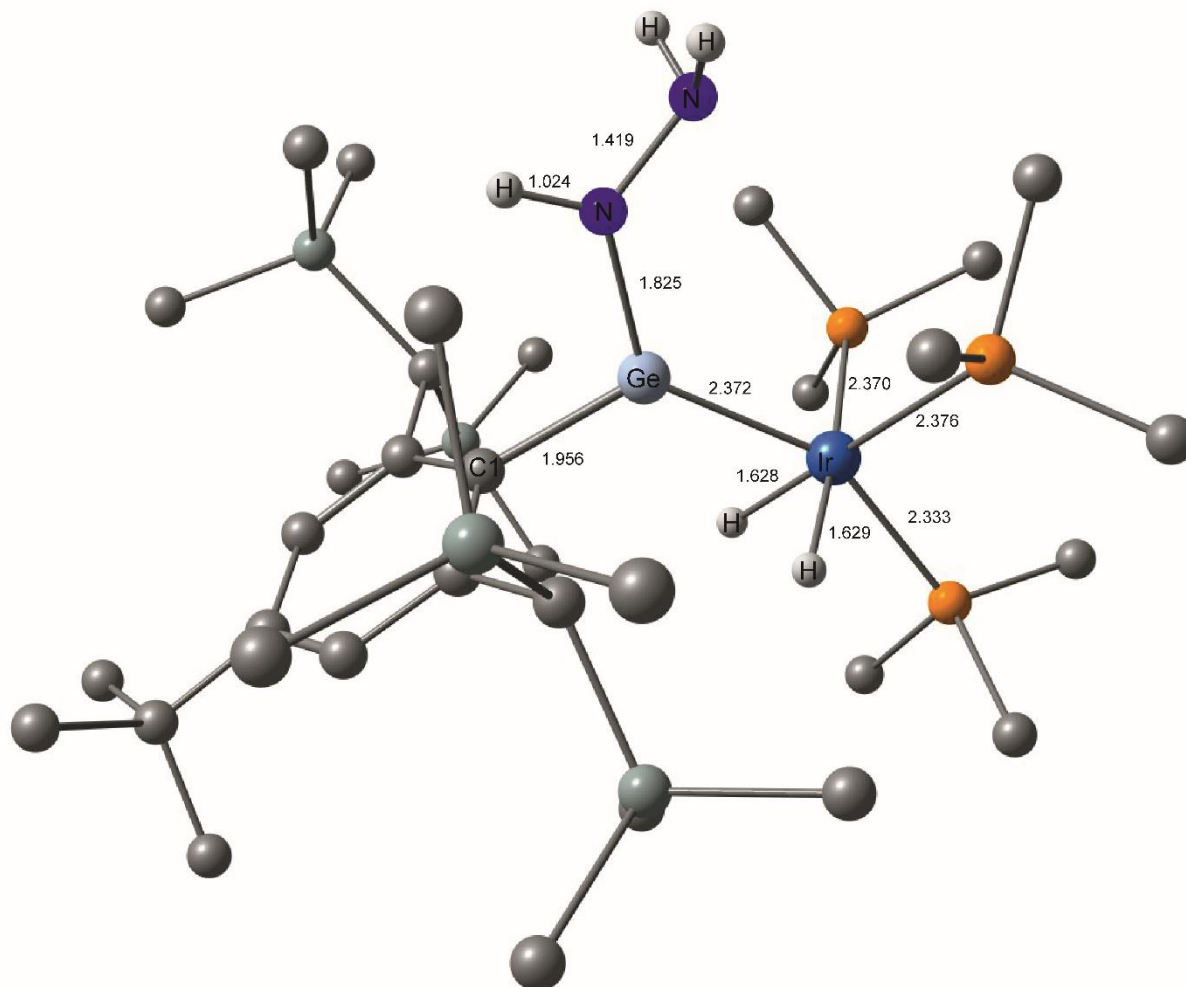
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P	3.42261769799964	3.13289242007388	0.51162262049624
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Compound 7.



Angle C1-Ge-Ir: 126.8°.

125

Coordinates from ORCA-job bp86optfreq_hnumac

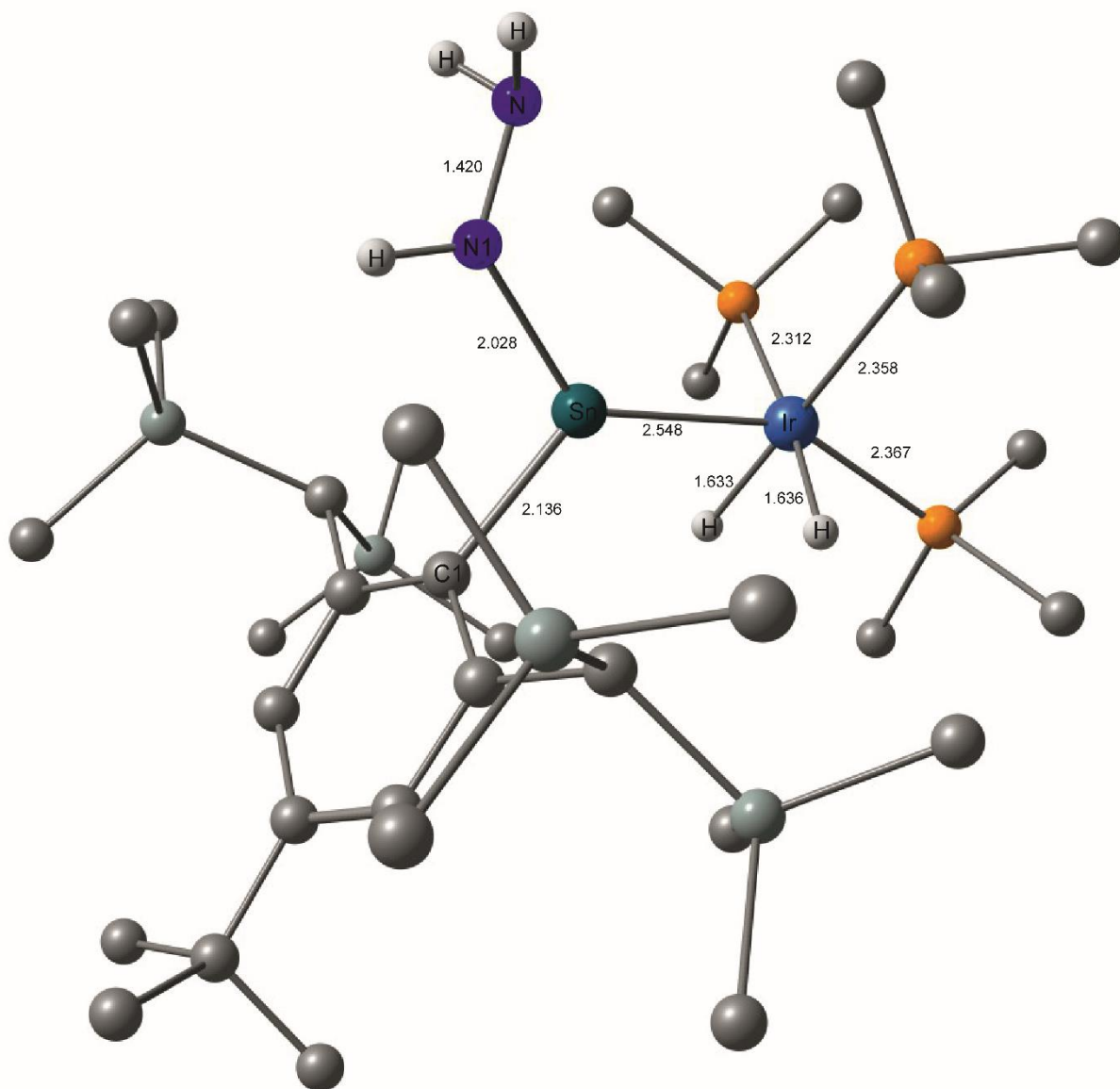
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Compound 8.



Angle C1-Sn-Ir: 127.3°

125

Coordinates from ORCA-job bp86optfreq_hnumac

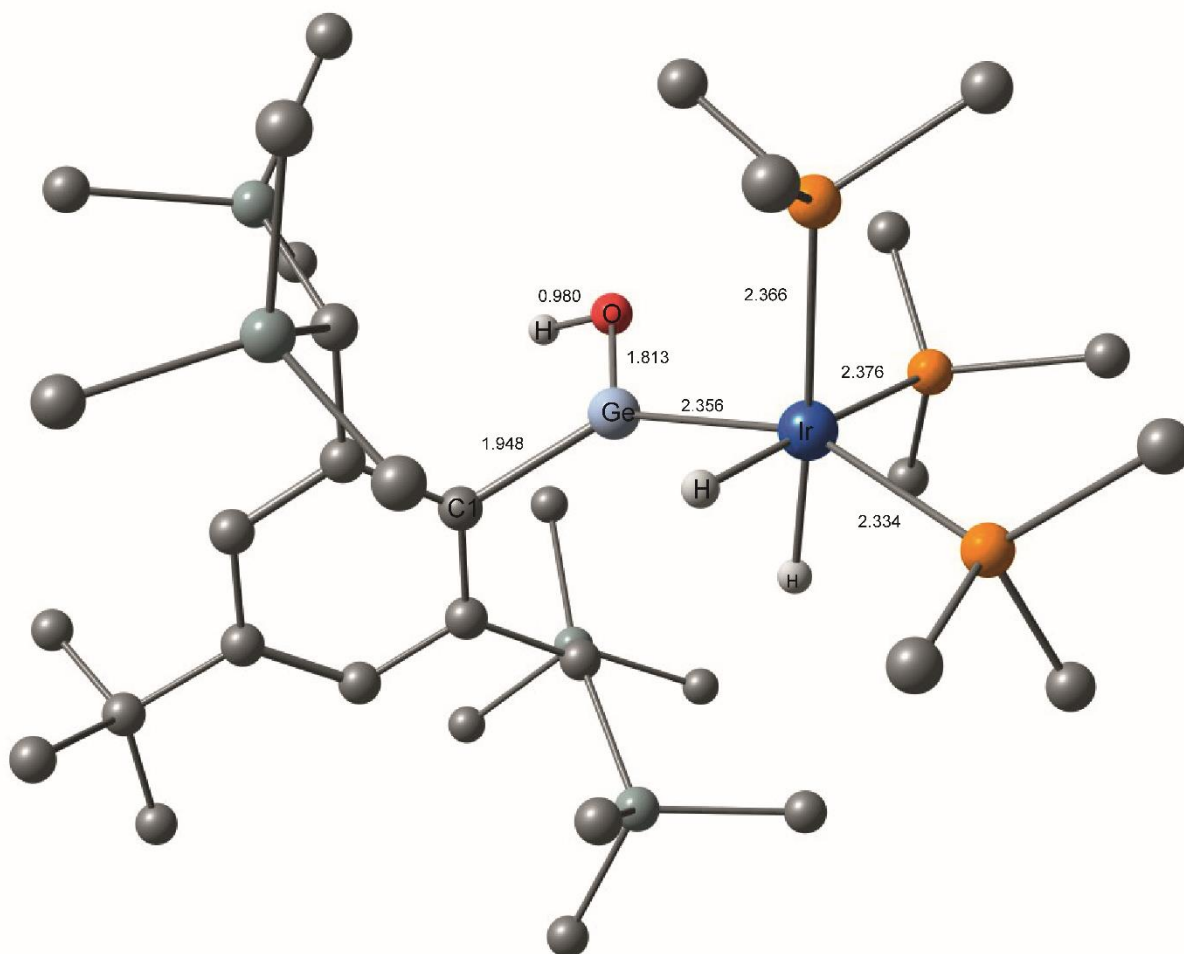
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Si	-0.41767329354608	3.44185283127140	-1.21053539681035
Si	3.07126387107707	-2.90052936138367	1.71705405296212
Si	0.66861155157628	3.69037274131888	1.90103976125856
P	-4.16100208158776	-0.18698352058013	-2.31678079542194
P	-3.45676779278239	-2.86480521076020	-0.09906820447785
P	-4.42339958423182	0.28125471536380	1.27674151937048
Sn	-0.84839083741963	-0.44902890152058	1.03773496655946
Ir	-2.96319589473310	-0.57554012010465	-0.37778537480977
H	-3.80427790179438	-0.41684039123585	-4.75189267573412
H	-5.13106611937981	1.69664670055414	-3.58094146757326
H	0.62589732458170	-2.68427695519217	-3.46312035654976
H	3.25140721298914	-4.26773017588491	-2.93715378918129
H	-2.27553653896636	-0.06748428980082	-3.84291974703266
H	-6.23753980482275	-0.69809659162373	-3.54677773919000
H	-0.81087304211710	2.53809808275692	-3.52783259228329
H	-3.61476060009827	2.14563942357013	-2.70097409709313
H	0.41752204753961	-5.29094453469203	-1.88051284891588
H	3.88032666227642	1.46985805320937	-3.51555712425567
H	1.36463496000336	-1.22143272473300	-2.72502567856708

H	5.30193000516243	2.55776133967634	-3.37302380404415
H	-2.97026863512652	-1.71708371233329	-3.80549636072684
H	-5.15362154062360	1.99790860082211	-1.79910655980478
H	0.23578140887092	5.39113519877520	-2.62615727284984
H	-0.19759028128016	-1.83050664826256	-2.11120362939427
H	0.70967668466536	1.88717887049980	-2.82707628207104
H	4.03309218247797	-2.84805476092526	-2.18074164714834
H	3.94555286547842	-4.40715225448241	-1.29381577568175
H	5.31992121312246	-0.38656530014891	-2.46509901998098
H	3.71950017723156	3.05778555841872	-2.70190737149518
H	-0.86346833842843	1.22839817634172	-2.28568882257432
H	-0.23786660351912	-4.56778619856425	-0.37977380154902
H	-5.63132078907953	-2.12243770950843	-2.63042648449609
H	-2.62086771713076	4.45000375798503	-1.87230781052050
H	-6.47545123195291	-0.79298361522415	-1.76071738870216
H	6.67044500273377	0.76922050813947	-2.28423834480906
H	1.68234898858228	4.70509139643432	-1.83076699488852
H	1.26303691208015	-5.53616751699412	-0.32285241317436
H	-3.60326478091728	-3.62424794098902	-2.41616736053636
H	0.55539204021128	5.74789732225234	-0.90180610520262
H	-1.81338791782869	-1.02024164970900	-1.44830162394692
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H	4.03459270443359	-1.06584660236151	-0.76702264132462
H	6.08232004217749	-0.13466553838402	-0.85872852706556
H	-2.47310896159091	0.96292242178839	-0.63839683613465
H	6.40938001705766	2.93020105736302	-1.06711176494996
H	-5.84635777380835	-3.02406692286608	-0.64165806393461
H	-6.18881243597276	1.36523927009969	-0.05082889470772
H	5.14924109095578	-3.09522949095725	0.27988680336482
H	-2.31172591725635	4.72235305362782	-0.12977053305375
H	2.63569685666575	3.02611238275472	-0.71708117356010
H	-1.92210490888926	-3.70217100061570	-1.80044937538118
H	-6.66627364217185	-0.28350612252625	0.48352411718903
H	3.04691462879624	-5.36299432538799	1.16498137681822
H	4.83180760156796	3.43856180983902	-0.39304238742720
H	-3.11212759157895	-4.98631516689298	-1.34083080035900
H	0.87072219464231	-2.38351395524597	0.85943117071702
H	2.26252001692075	5.26658325795540	0.72940388863209
H	5.16365114694818	-1.58632064646596	1.25285100570780
H	5.74655349609074	2.10894513411862	0.38537689504526
H	-5.28605093020475	-4.49762599473646	0.23450013389091
H	-6.73533936068125	1.09296968530165	1.64443683838684
H	-0.72325763432636	2.07328382384943	0.76839680910529
H	-5.58098821052492	-2.96349125450239	1.12855309025916
H	1.65020093880206	-4.93010820829590	2.20506574941987

H	5.52142887511470	-3.15908228336503	2.03010427844793
H	-3.71427966959522	2.62369438946516	1.15569187239657
H	-0.83414954135883	5.66716237447765	1.44533032672673
H	3.28841619974511	-5.08446847196339	2.91402153242746
H	3.14010333565824	3.91847616097446	1.52684940573134
H	2.49346724289895	5.27170664936106	2.50516256672015
H	-5.19625285653274	-1.65319092367156	2.57000773804621
H	-4.56309983671865	2.29367416248409	2.72118794699952
H	-1.49817755001602	-3.63942176274555	1.13090924235573
H	-1.71207427054415	4.39113823951110	2.35248422983154
H	-2.89009980593064	-4.75274488280879	1.41788633811025
H	-2.86546366827068	1.73555559629936	2.46009272383728
H	2.71704590105776	-0.83504866051906	3.09968020418843
H	0.36607448414667	-0.61835993430875	3.41364707341622
H	-2.80989252068415	-3.13343936259569	2.23980064994506
H	-0.54446993137784	5.45494363138625	3.19706651815997
H	1.74411792347968	-2.21318904804162	3.74240806709661
H	-5.26412924926724	-0.15073460022422	3.55562067920708
H	-3.66988464494767	-0.96869851250434	3.23081150823982
H	3.50082994993166	-2.12143682869931	4.07300581536520
H	1.65445609205226	1.76180466684961	3.15586737959792
H	-0.06767322076047	1.98359332727079	3.60350690827017
H	1.18514291739730	3.07450617913182	4.28718483817419
H	-1.62733332202618	-0.73289459392213	4.73252731930403
H	-1.17520016000664	-2.24175090190638	4.24832178523679

Compound 9.



Angle C1-Ge-Ir: 133.1°

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Coordinates from ORCA-job bp86optfreq_hnumac

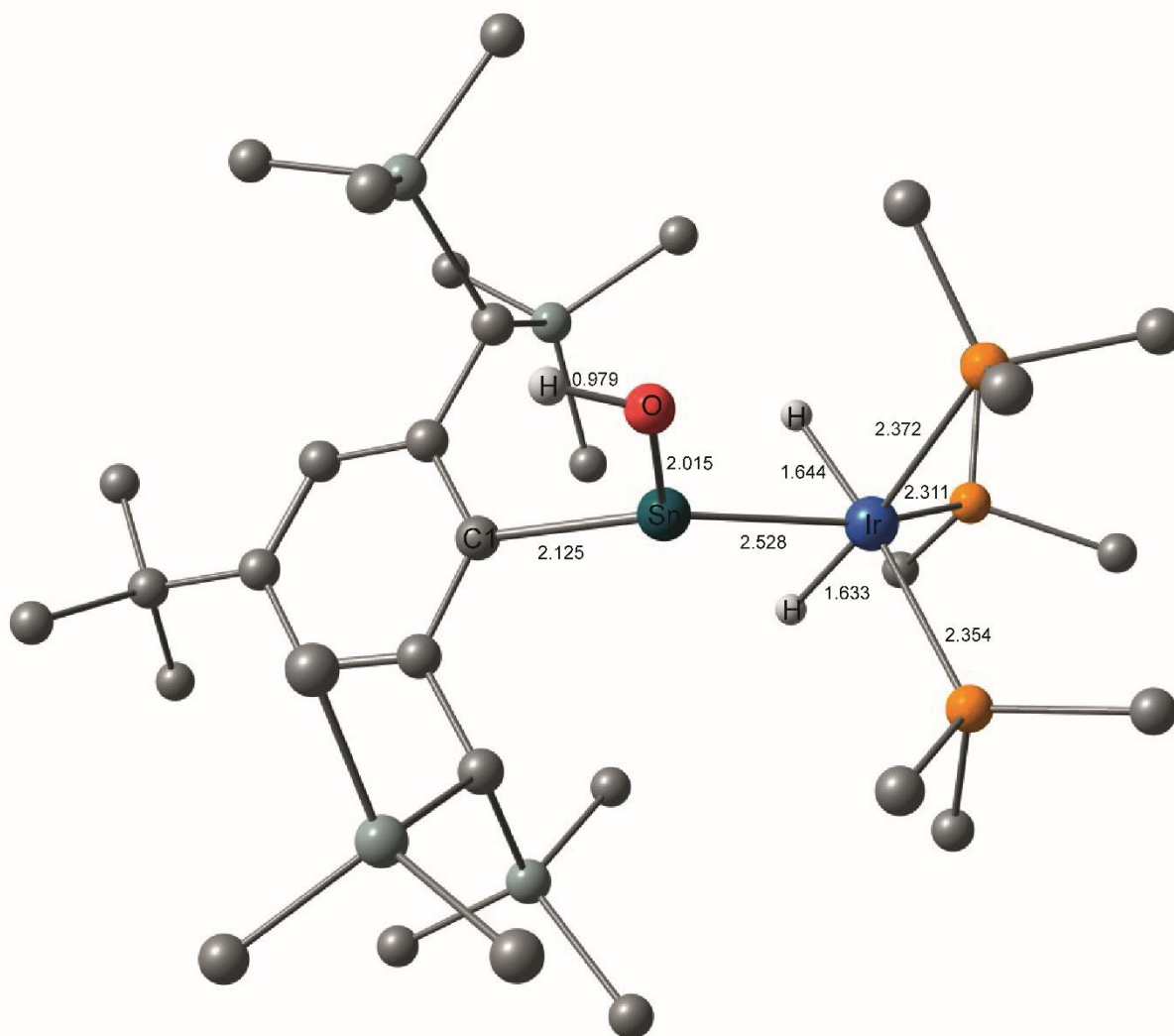
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C	-3.18980210605328	2.11361100456462	-3.37499573570355
C	0.66284561740400	0.99544138265616	-3.26468468636151
C	0.36534744372747	4.09203889810469	-3.12161505274028
C	3.15242234871614	2.75729297259247	-3.08656527917527
C	-5.48282812338105	-1.21677652071963	-3.07941651365468
C	-4.18743069041875	-3.39348296856436	-1.72095948007758
C	-5.41744221156956	2.13014897232947	-1.55656507092466
C	0.57246351497419	-3.05309090953660	-1.42270659287042
C	5.67101104267589	-0.36226158691499	-1.25640050189013
C	-2.91773641565862	3.27499401409901	-0.76054588414484
C	1.16421136659168	2.44741988802654	-0.61690728030777
C	3.23820160931931	4.77740079315344	-0.07518165332988
C	3.13890218692190	0.91341068426713	-0.15451058607588
C	1.75432492424402	1.15795730348001	-0.10511695159209
C	5.21881545856035	-0.51013297791953	0.21623636159394
C	0.20571725686111	5.18920890645026	0.44456514096465

C	3.69747334788960	-0.30128552269253	0.29964434810938
C	1.81497156447855	-4.90758877423956	0.73035598326245
C	0.92008640359491	0.15908331054196	0.45258555342690
C	-6.05601968387437	-0.97307548408495	0.68652802248136
C	-1.25134271821246	-4.48284984155448	0.61945421990187
C	5.64165579601208	-1.90219885787010	0.72157446258920
C	2.83286805525877	-1.27953788912721	0.82416720552177
C	1.44036439326134	-1.06637186990138	0.92435299266122
C	5.91471556805678	0.56506516677352	1.08603206650935
C	0.52959637881954	-2.11992868677019	1.50078302940314
C	-4.54513484689848	1.03132068922503	2.07078655253928
C	1.84875071283421	3.32374028163070	2.26434751641273
C	-3.76716750218028	-1.71848705313046	2.27515267839176
C	2.57929449233313	-2.89269937396709	3.79370594311640
C	-0.41690131863416	-3.62882956065387	4.04645322929175
C	0.49170815613671	-0.66825412874195	4.18325470942103
O	-1.30527124704253	1.38291633750872	2.05778634712000
Si	1.35683146434964	2.59182446337897	-2.52407095877036
Si	0.43911322234967	-3.66556754648881	0.36322855249704
Si	1.63611116824302	3.95107329949863	0.48984130263658
Si	0.81543288542641	-2.35565208601858	3.38293739955591
P	-3.86064564722304	-1.68835227858515	-2.33396478171487
P	-3.60203523821582	1.78759166717055	-1.60805633600950
P	-4.31023353194045	-0.47218201157314	1.02940612739256
Ge	-1.00179977288776	0.46964185887711	0.52080967771956
Ir	-2.80244630956859	-0.28594031241645	-0.79674394225461
H	-3.30021659804660	-2.70278465615484	-4.51813874954617
H	-2.61276385866646	-1.03660078814425	-4.32657628590564
H	0.68957587347025	1.02156075210389	-4.37361553647271
H	0.33209592104952	4.11431845046757	-4.23064499360185
H	3.17329063923583	2.91671941944064	-4.18510935654664
H	-3.66465389119862	1.34478066855576	-4.01506003262632
H	-3.53181981153119	3.11689650373330	-3.69792808376632
H	-1.84449102440660	-2.41114033401344	-3.47652031846527
H	-5.83410331256093	-2.00045985254175	-3.78029193484485
H	-2.09348121625725	2.03675572431241	-3.50410066387087
H	-5.37677466552979	-0.26639018023607	-3.63699183489133
H	-0.38100951916923	0.80363367722419	-2.94145176823843
H	-0.68119046287444	4.07965733979968	-2.75468761265170
H	1.26528466162153	0.12726967025780	-2.92666501734296
H	3.72254871132387	1.83057041495877	-2.87645434852965
H	0.82785758857672	5.04239072700989	-2.78513162139624
H	-4.65865234759329	-4.01685071803339	-2.50665399005281
H	3.67978759631790	3.60701911826755	-2.61236495071359
H	-5.96909394201335	1.34316227379621	-2.10263246506168

H	-6.23890552490673	-1.07993717269568	-2.28340564938025
H	-5.64794355755577	3.11496216761565	-2.00981840872015
H	0.41871636514452	-3.88271050618324	-2.14360947106293
H	-1.64843765352411	-0.24194755205788	-1.94590229440464
H	-3.22671017295652	-3.84724461990782	-1.41345250581422
H	5.16505971997342	-1.10719964631856	-1.90378100654644
H	5.44691040584417	0.64593996925397	-1.65862333347066
H	1.57072354969490	-2.61045749135090	-1.61461402735786
H	-0.18530586761439	-2.26639905517297	-1.61671561822064
H	-3.35176672713700	4.21558457870156	-1.15454335892559
H	6.76567038408817	-0.51890517385956	-1.34224053787348
H	3.13712664225431	5.23186392501212	-1.08137373355647
H	-1.82170592894465	3.29372511420433	-0.91139677129020
H	-4.84995693377050	-3.36181101001518	-0.83527579717031
H	-5.76467942203472	2.13471454328488	-0.50564459946625
H	-0.01644868036373	5.53960051601304	-0.58301265492630
H	0.04709372072203	2.40185868812191	-0.49838411420086
H	3.79660434986114	1.69395859590468	-0.56143477945091
H	4.08522447716191	4.06212235887634	-0.10225301222357
H	1.75650282425934	-5.76061356397335	0.02270466727534
H	-2.13658040537485	-1.71156814290706	-0.34915490739676
H	-1.40236453717448	-5.30763704458518	-0.10764156753047
H	-6.52475602438811	-0.23137832318783	0.01152543813576
H	-3.10709048852916	3.20016929370847	0.32711615168395
H	-6.07828328206086	-1.96217212185599	0.19035310495880
H	3.50929022481048	5.58835311722984	0.63230943930237
H	5.18138131216809	-2.71517100133953	0.12391796987251
H	2.81968528327223	-4.45172460473438	0.61891464534814
H	-2.05506744055140	-3.73387508066204	0.46425338375221
H	-0.71610152799787	4.73573323519763	0.86420978607002
H	6.74134049804752	-2.01347756063654	0.64210307910145
H	5.67619241914226	1.59092787457842	0.74042170190293
H	0.44677685834781	6.08119347731311	1.05917776972905
H	7.01653639064277	0.44344562397603	1.04468586899446
H	3.23885621957420	-2.23570087722727	1.17417582856283
H	1.73487769049323	-5.31869221960818	1.75715240867168
H	-6.64710495409083	-1.03105862383825	1.62234918501879
H	-5.00430678273413	1.83862186152771	1.46835637688816
H	-1.36688996598749	-4.90334909574887	1.63738053492438
H	-0.52811806648311	-1.74841030538687	1.46770252964357
H	-3.63883870044815	-2.70160139940272	1.78340411332173
H	5.36889329917391	-2.05763753791370	1.78492774990596
H	5.59894435991983	0.48254074750757	2.14596053832579
H	2.56269810508596	2.47700031904536	2.31359525736419
H	-3.55116892522758	1.37303345632209	2.42011586184636

H	0.87745265112521	2.98619424176683	2.68270829327322
H	-2.78300166117996	-1.40399042335853	2.67505018896873
H	-0.47038415738917	1.49836224446173	2.55849761418176
H	2.22278161634954	4.13185539329947	2.92591075726473
H	-5.20021410710371	0.81728600927216	2.93883317061167
H	-4.48799703418030	-1.80895262786100	3.11177193442112
H	2.88164765585340	-3.80943956600397	3.25015181930200
H	3.30854901481096	-2.09256572932687	3.55727515747405
H	-0.18950913593585	-4.64884465239663	3.67499997187083
H	-1.45957039844879	-3.38427487550227	3.75737058585388
H	1.15300184283517	0.10136274506189	3.73113331470888
H	-0.56266850707552	-0.34959109047636	4.04839671369365
H	2.65466426378176	-3.10469138164649	4.88072974959966
H	-0.37378730272942	-3.66188260809077	5.15482043518524
H	0.70019356516005	-0.69140518333687	5.27261502293688

Compound 10.



Angle C1-Sn-Ir: 135.5°

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Coordinates from ORCA-job bp86optfreq_hnumac

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C -3.22160861310404 2.04316252724655 -3.49829711448996
C 0.70140257814807 0.93476205242331 -3.16673456422190
C 0.35440849934028 4.02141843056167 -3.11716193143474
C 3.17072950968396 2.76343876095499 -3.07393552000901
C -5.61217449948575 -1.26161269575057 -3.12087732409057
C -4.44622319787447 -3.38639265418812 -1.56708583002925
C -5.50960925546636 2.18749805298967 -1.75342182458198
C 0.57758676800681 -2.85849529676538 -1.41361584235052
C 5.76369544784113 -0.30608088884032 -1.27463243259315
C -2.99905104918354 3.27183519826345 -0.91047645165165
C 1.23317107974877 2.45207043071493 -0.57616258575558
C 3.34279113755623 4.70400528022043 0.11135366698393
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C	5.34718382603324	-0.44319258683611	0.20958087311872
C	0.29737148833456	5.26214147217666	0.33418914773113
C	3.82534026503843	-0.25148955347315	0.32641775564943
C	1.88344503034466	-4.86155085060629	0.56103811769489
C	1.05611352024683	0.17757816608822	0.53811777685009
C	-6.29506906347225	-0.76036031243702	0.61003713709656
C	-1.18586750544225	-4.37483770102129	0.60506462521409
C	5.79923863955584	-1.82455947281351	0.71910671488806
C	2.98548035316683	-1.23884425745183	0.87562501476394
C	1.59229352498790	-1.04034582248748	1.00391864018433
C	6.05077282917337	0.64889729796534	1.05164141115933
C	0.69400747243537	-2.11457544912973	1.56592473928304
C	-4.68533847829622	1.17402466193340	1.98635210476943
C	1.64156385144906	3.33034786718589	2.31899432451762
C	-4.07066270392125	-1.61624239253765	2.23724214196474
C	2.81230441849919	-3.08510346072975	3.72496475437845
C	-0.19398304859130	-3.76426744164643	4.03780143089564
C	0.79193516202901	-0.84479364554835	4.34052963173546
O	-1.47164971227477	1.00158769648665	2.48580795288536
Si	1.38665608533001	2.56272906465369	-2.48788454601676
Si	0.51399502878912	-3.58130055492433	0.33438729456993
Si	1.65900384504056	3.96251667408393	0.53625840778372
Si	1.04888344431944	-2.48008921410972	3.41829423891675
P	-4.03339057249022	-1.74705810536588	-2.29784832729562
P	-3.70729556591402	1.78098261430425	-1.73966494455182
P	-4.52677524303866	-0.35665026645921	0.97088075238297
Sn	-1.05126654953245	0.44237329657230	0.59637092633521
Ir	-3.00072651968865	-0.27746656504470	-0.84354970037896
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