

SUPPORTING INFORMATION

**Oxidative Addition of SiH_4 and GeH_4 to $\text{Ir}(\text{PPh}_3)_2(\text{CO})\text{Cl}$:
Structural and Spectroscopic Evidence for the Formation of Products
Derived from *Cis* Oxidative Addition**

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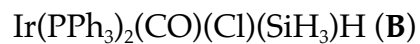


-3042.89300853456 Hartrees

Atom	x	y	z
C	13.881313	-6.751043349	1.748774101
C	11.55271394	-9.703181827	3.575549246
C	10.44011991	-10.40702412	4.06454381
C	10.37560916	-11.79622437	3.95248779
C	11.41349789	-12.50103448	3.342961321
C	12.51742234	-11.80968403	2.843624176
C	12.58839102	-10.42219166	2.96131749
C	10.70313743	-7.343219768	2.118796919
C	10.77902616	-6.006414328	1.689628666
C	10.06840865	-5.586124761	0.565096742
C	9.284091081	-6.488601516	-0.155199101
C	9.210391603	-7.817428409	0.261161804
C	9.910639376	-8.24354572	1.391474703
C	10.51489098	-7.386459261	5.017663269
C	10.59831159	-8.043664436	6.256824401
C	9.783379723	-7.656832862	7.31954142
C	8.876123537	-6.608680819	7.164930137
C	8.788172985	-5.95041777	5.939664475
C	9.600537749	-6.333417556	4.87315378
C	16.23344305	-4.784081319	5.359834546
C	16.62548482	-5.327353684	6.5949652
C	16.73925395	-4.51485207	7.722779339
C	16.46134804	-3.150348897	7.640196106
C	16.07087342	-2.603872648	6.418321637

C	15.95597794	-3.411056189	5.286934412
C	16.33409569	-4.743994876	2.450430121
C	15.30386989	-3.911807972	1.976658642
C	15.53199068	-3.04787789	0.905468151
C	16.77973711	-3.007814371	0.281249402
C	17.80312544	-3.835575345	0.741471417
C	17.58612574	-4.695306008	1.820168964
C	17.45705566	-7.001225796	3.891338323
C	17.3747361	-8.240916045	3.240929932
C	18.48401939	-9.083782751	3.172850275
C	19.69261664	-8.704337804	3.757593864
C	19.78691014	-7.471219566	4.403787136
C	18.68097496	-6.622719868	4.467313517
Cl	12.79432337	-4.728278544	4.356132843
H	9.623198621	-9.872773274	4.537667514
H	9.511242766	-12.32598959	4.343543366
H	11.3623498	-13.5831419	3.258821899
H	13.33018377	-12.35012487	2.366332904
H	13.45486281	-9.892863888	2.580498376
H	11.38577363	-5.296412429	2.246223069
H	10.13385696	-4.548032752	0.250570007
H	8.738134467	-6.159737389	-1.035155263
H	8.607588617	-8.531202164	-0.293942063
H	9.838856347	-9.281495963	1.697229058
H	11.29539068	-8.861611266	6.396171149
H	9.861734746	-8.177985718	8.269682167
H	8.242293961	-6.307386427	7.994527704
H	8.086492363	-5.131435	5.807997733

H	9.517380503	-5.80611241	3.930867392
H	16.84428178	-6.385160223	6.682051842
H	17.04426618	-4.955373803	8.667994115
H	16.54720472	-2.519498601	8.520500297
H	15.84843048	-1.543338661	6.339849994
H	15.646027	-2.964245806	4.350495945
H	14.32758735	-3.937800786	2.454606035
H	14.72546163	-2.408998946	0.555800832
H	16.95129934	-2.340756609	-0.559033082
H	18.77733449	-3.818468018	0.260260741
H	18.39614933	-5.331435073	2.159519989
H	16.43618439	-8.54839335	2.793208005
H	18.39845467	-10.04152513	2.666964601
H	20.55404202	-9.364637729	3.711855195
H	20.72322115	-7.16497662	4.862161815
H	18.77224345	-5.66649702	4.971720656
H	14.51042212	-8.359132325	3.507668755
Ir	13.85043427	-6.930918225	3.685355543
O	13.99925166	-6.861990691	0.606267944
P	11.63964703	-7.861224578	3.633189593
P	15.99657149	-5.870322095	3.884824147
Si	14.12239459	-7.79003007	5.976460505
H	15.54581713	-8.118048524	6.300119082
H	13.64507948	-6.917404019	7.086852687
H	13.4449316	-9.109394932	6.177522768



-3042.89895749938 Hartrees

Atom	x	y	z
Ir	3.468649698	-5.486707167	-14.5622031
Cl	1.37626713	-4.561481481	-13.41574103
Si	5.268959474	-5.635922115	-16.14756131
P	4.675677176	-4.025403248	-13.08991008
P	1.941084195	-6.714521768	-15.95039002
O	4.330376649	-8.017393852	-13.02556766
C	3.940800501	-7.060612789	-13.54461621
C	6.493765644	-3.865635578	-13.3786635
C	7.115474822	-2.636774551	-13.63109826
H	6.527526004	-1.725895838	-13.66487491
C	8.495209354	-2.573550619	-13.844285
H	8.961451822	-1.612445943	-14.04329414
C	9.26965754	-3.73128668	-13.80088545
H	10.34175868	-3.679172768	-13.96780327
C	8.657184177	-4.960862375	-13.54485566
H	9.250211187	-5.870438583	-13.51182408
C	7.281214314	-5.029060243	-13.33918419
H	6.818776836	-5.993881397	-13.15046259
C	4.635054876	-4.547834905	-11.3132578
C	3.504732119	-5.191043603	-10.78462161
H	2.641468282	-5.36361924	-11.41868452
C	3.475056088	-5.572851856	-9.442826559
H	2.591692731	-6.069641626	-9.050911095
C	4.564570392	-5.320254095	-8.60892548
H	4.538453241	-5.622837522	-7.565703636

C	5.688635851	-4.674192365	-9.124772496
H	6.543522464	-4.469276398	-8.486044511
C	5.725888696	-4.290231497	-10.46540385
H	6.610923638	-3.794095261	-10.84890939
C	4.052149865	-2.294295383	-13.1001111
C	3.815116605	-1.655127167	-14.32694223
H	3.963302075	-2.19701839	-15.25493683
C	3.369803871	-0.335507767	-14.35946922
H	3.189147184	0.14659186	-15.31632728
C	3.140806435	0.35791916	-13.16920906
H	2.780817322	1.382858001	-13.19583647
C	3.366961555	-0.273295283	-11.94742961
H	3.181896975	0.256160364	-11.01688512
C	3.824558852	-1.591218898	-11.90997327
H	3.990991923	-2.071891701	-10.95224985
C	0.594797304	-5.692363942	-16.67499061
C	0.888097734	-4.414734443	-17.1740037
H	1.890825119	-4.01458357	-17.07266843
C	-0.106416094	-3.649606254	-17.77940087
H	0.134609397	-2.660912135	-18.16016737
C	-1.408137432	-4.143760611	-17.88187608
H	-2.185434957	-3.54156242	-18.34450137
C	-1.708780561	-5.409341429	-17.37986608
H	-2.721236352	-5.797877901	-17.4476654
C	-0.713310866	-6.183470381	-16.782495
H	-0.961322362	-7.165685141	-16.39489859
C	1.072468397	-8.102069313	-15.07895213
C	0.667724015	-7.953789252	-13.74236879

H	0.856215514	-7.017373684	-13.22680259
C	-0.000324772	-8.990784208	-13.08985086
H	-0.306338579	-8.857984487	-12.05562154
C	-0.276119126	-10.18647908	-13.7537856
H	-0.792687221	-10.99280617	-13.24029216
C	0.115205501	-10.33937916	-15.08392742
H	-0.095822415	-11.26434437	-15.6138775
C	0.782855508	-9.306425086	-15.74354858
H	1.080368478	-9.44640319	-16.77683988
C	2.67227459	-7.58574529	-17.40206812
C	3.682927295	-8.534901749	-17.17448794
H	4.019961394	-8.741019035	-16.1624991
C	4.264392816	-9.21737081	-18.23964349
H	5.045248214	-9.94790012	-18.04785206
C	3.851415359	-8.956722936	-19.54854659
H	4.310447291	-9.484291404	-20.38009381
C	2.852755042	-8.013727786	-19.78265517
H	2.526886952	-7.804090017	-20.79784743
C	2.261679567	-7.332779403	-18.71580764
H	1.482696832	-6.603934251	-18.91199562
H	6.134108702	-4.422213155	-16.14579819
H	6.197626699	-6.791538422	-15.9417637
H	4.789383702	-5.751364918	-17.55356504
H	3.264677097	-4.213828009	-15.55439209

$\text{Ir}(\text{PPh}_3)_2(\text{CO})(\text{Cl})(\text{SiH}_3)\text{H} (\text{C})$

-3042.88125086244 Hartrees

Atom	x	y	z
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Ir	3.440216996	-5.335485366	-14.68581955
Si	5.10600221	-5.057836017	-16.52401041
P	4.672132621	-4.001532745	-13.09881264
P	1.976371305	-6.748294225	-15.97337799
O	4.662908235	-7.81071075	-13.49376748
C	4.194464284	-6.852523247	-13.95588562
C	6.515096757	-4.018491817	-13.27927755
C	7.2910756	-2.885241475	-12.99011266
H	6.812442491	-1.959688042	-12.69063772
C	8.682471818	-2.933945547	-13.08847286
H	9.265698709	-2.044281356	-12.86718444
C	9.320808162	-4.113664681	-13.46831016
H	10.40390716	-4.148918256	-13.54771668
C	8.559466925	-5.248010475	-13.75017652
H	9.044176681	-6.172378662	-14.05138088
C	7.169461048	-5.200959694	-13.65937653
H	6.601960341	-6.092710765	-13.89384182
C	4.429000218	-4.6426534	-11.37541194
C	3.137720746	-4.970398109	-10.92916289
H	2.297127118	-4.868595118	-11.60787601
C	2.931022564	-5.434097554	-9.630563755
H	1.923926781	-5.678145856	-9.303217755
C	4.009934939	-5.593570012	-8.758294716
H	3.849587041	-5.967250554	-7.750748075
C	5.295637619	-5.273958227	-9.192765615
H	6.144018366	-5.396818474	-8.524935544
C	5.505254403	-4.795873377	-10.48802146
H	6.512677749	-4.549969329	-10.80495928

C	4.267375392	-2.212169361	-12.99333786
C	4.539612473	-1.393279793	-14.10195661
H	4.945160818	-1.824520929	-15.01056322
C	4.283678034	-0.025581831	-14.0405161
H	4.500335237	0.596947785	-14.90393684
C	3.739003525	0.539751025	-12.88508729
H	3.536137988	1.606304154	-12.84296625
C	3.454757437	-0.271259366	-11.78756286
H	3.031105389	0.158837953	-10.88414294
C	3.719879044	-1.641551751	-11.83732622
H	3.504261228	-2.257356301	-10.97097909
C	0.495539749	-5.948516483	-16.6967431
C	0.654834628	-4.987069893	-17.70852383
H	1.646720172	-4.716127064	-18.05179152
C	-0.461758917	-4.366034525	-18.26358317
H	-0.326912398	-3.624458265	-19.0457159
C	-1.7426709	-4.678049747	-17.80459307
H	-2.610170895	-4.183938821	-18.23376672
C	-1.90535425	-5.619495208	-16.78960296
H	-2.898754768	-5.865170215	-16.42431093
C	-0.792600261	-6.256374027	-16.23894745
H	-0.933023344	-6.991868483	-15.45432197
C	1.291951723	-8.138088735	-14.95497145
C	1.094261099	-7.992020547	-13.5743565
H	1.370295952	-7.060685267	-13.09208647
C	0.553422624	-9.034848632	-12.82106271
H	0.412675127	-8.905749717	-11.75135582
C	0.20396341	-10.23747567	-13.43349509

H	-0.210053659	-11.05125998	-12.84420801
C	0.39400781	-10.39266731	-14.80722536
H	0.126471662	-11.32679471	-15.29357927
C	0.932563645	-9.352892796	-15.56338099
H	1.078365231	-9.492415853	-16.62928539
C	2.750980473	-7.679805864	-17.37428214
C	3.947119343	-8.377201363	-17.137118
H	4.428736192	-8.325363846	-16.16680204
C	4.532422292	-9.146558437	-18.14035377
H	5.458069614	-9.677034026	-17.93557984
C	3.938881863	-9.229248039	-19.40154877
H	4.399015656	-9.824481249	-20.18518724
C	2.752495994	-8.540106801	-19.64711961
H	2.280034701	-8.596575566	-20.62406475
C	2.157974504	-7.774381993	-18.64114651
H	1.230135934	-7.253518019	-18.84910727
H	5.842114882	-3.758629065	-16.43903124
H	6.192730273	-6.090439229	-16.62408777
H	4.463251019	-5.06267521	-17.8730179
Cl	2.473120157	-3.294455	-15.69523773
H	2.167977997	-5.202973056	-13.63775742