Indirect Access to Carbene Adducts of Bismuth and Antimony Substituted Phosphaketene and their Unusual Thermal Transformation to Dipnictines and [(NHC)$_2$OCP][OCP]

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Supporting Information

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NMR Spectral Data

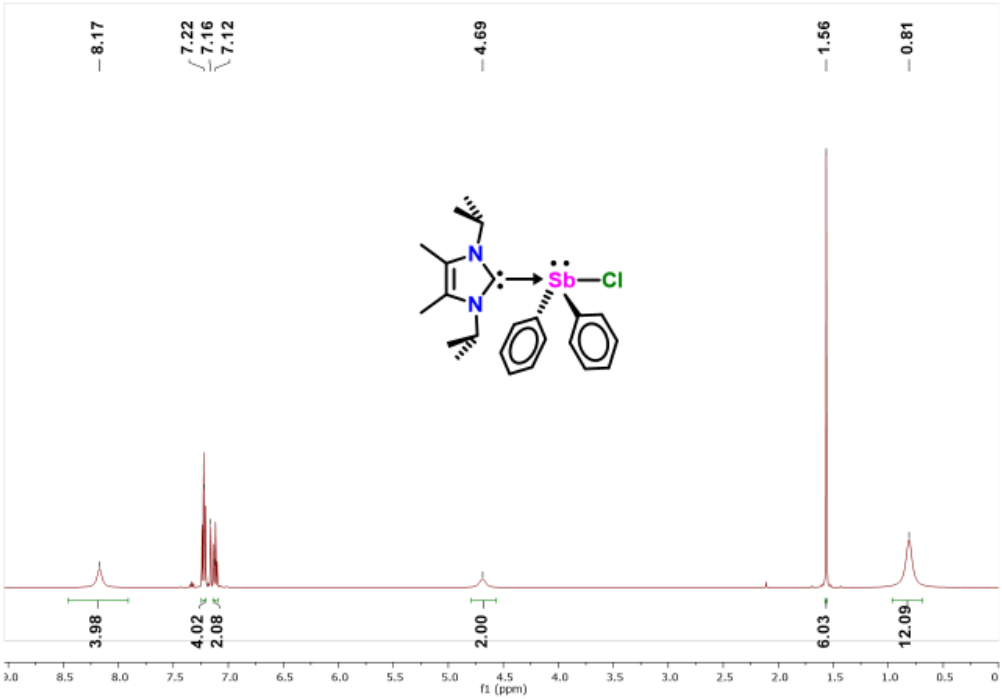


Figure S1: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of complex **1**.

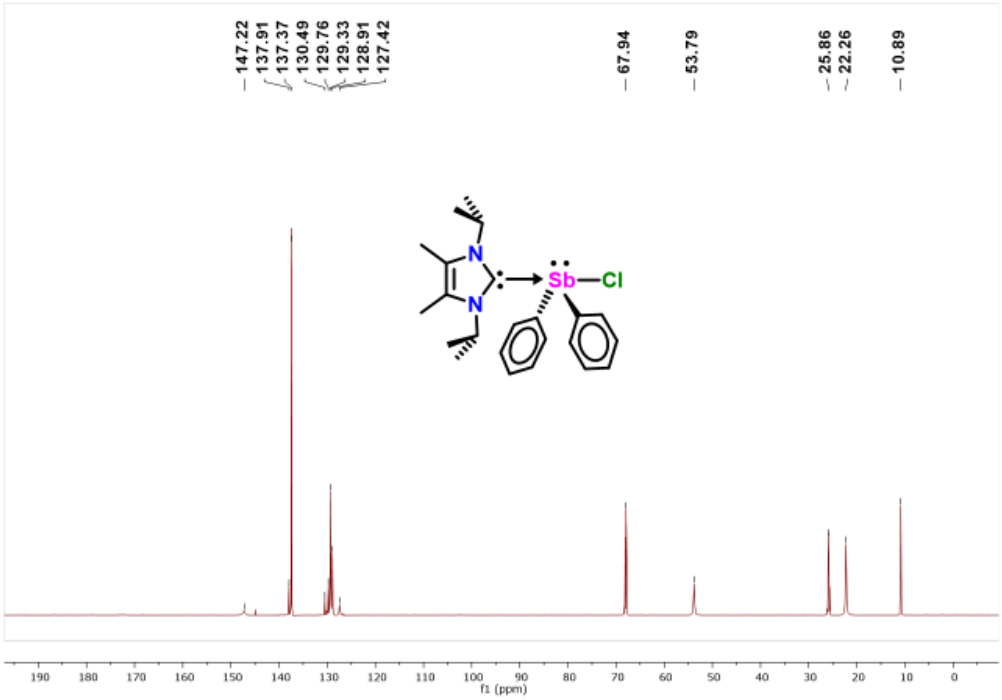


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum (201.19 MHz, C_6D_6, 298 K) of complex **1**.

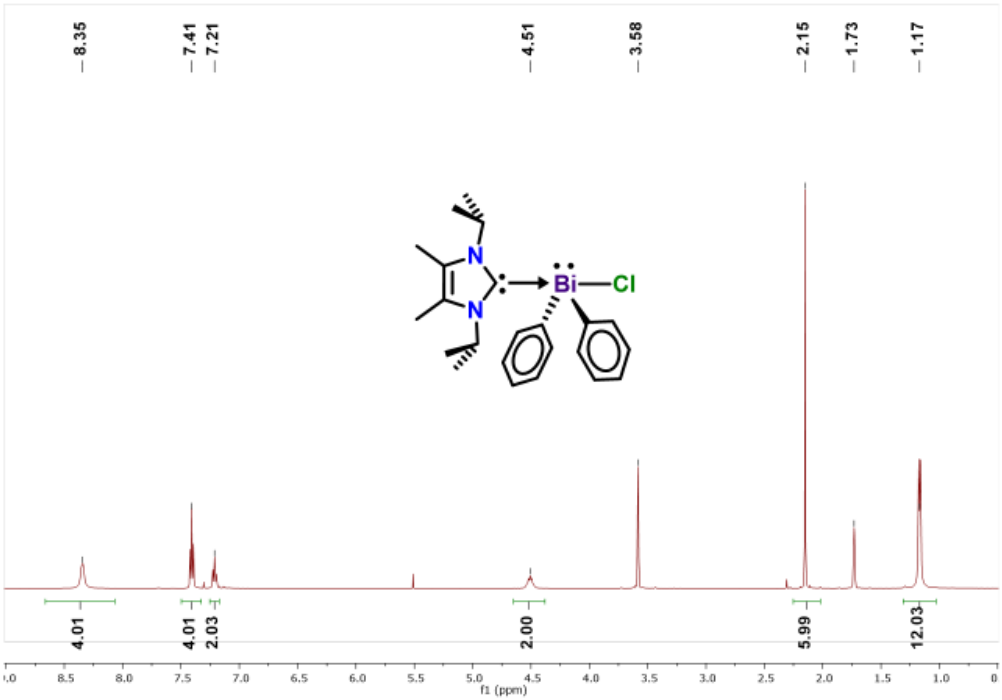


Figure S3: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of complex **2**.

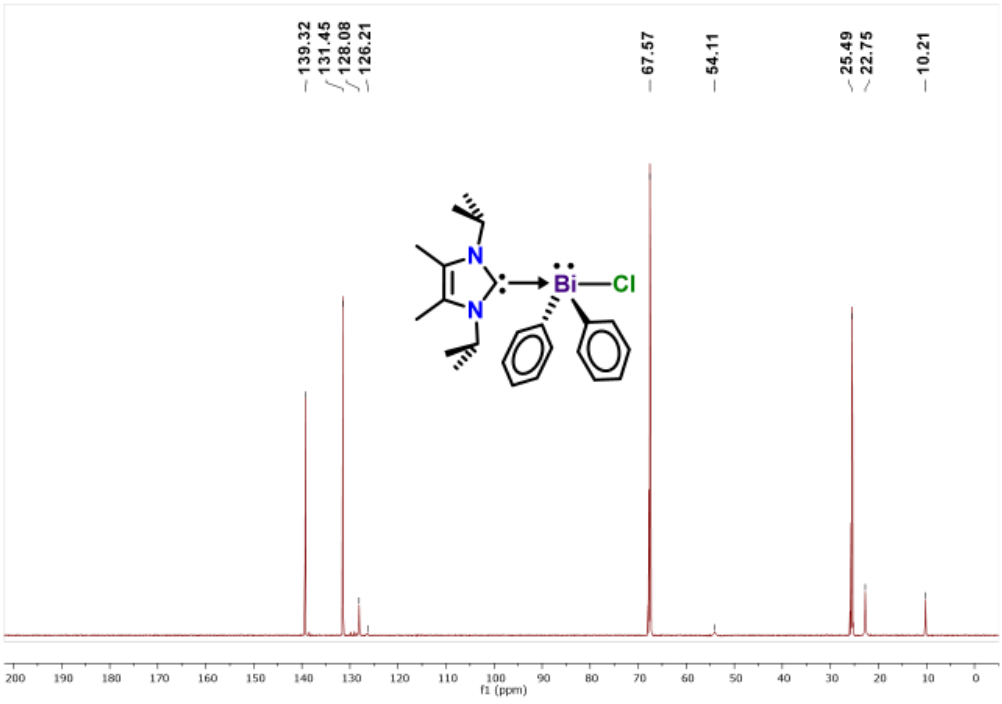


Figure S4: $^{13}C\{^{1}H\}$ NMR spectrum (201.19 MHz, C_6D_6, 298 K) of complex **2**.

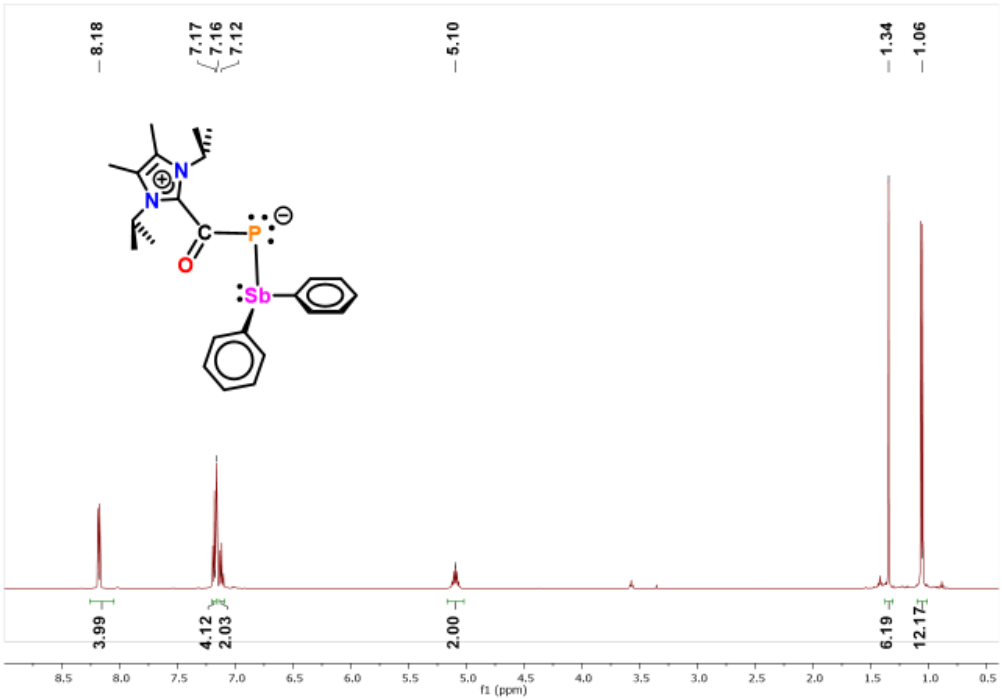


Figure S5: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of complex **3**.

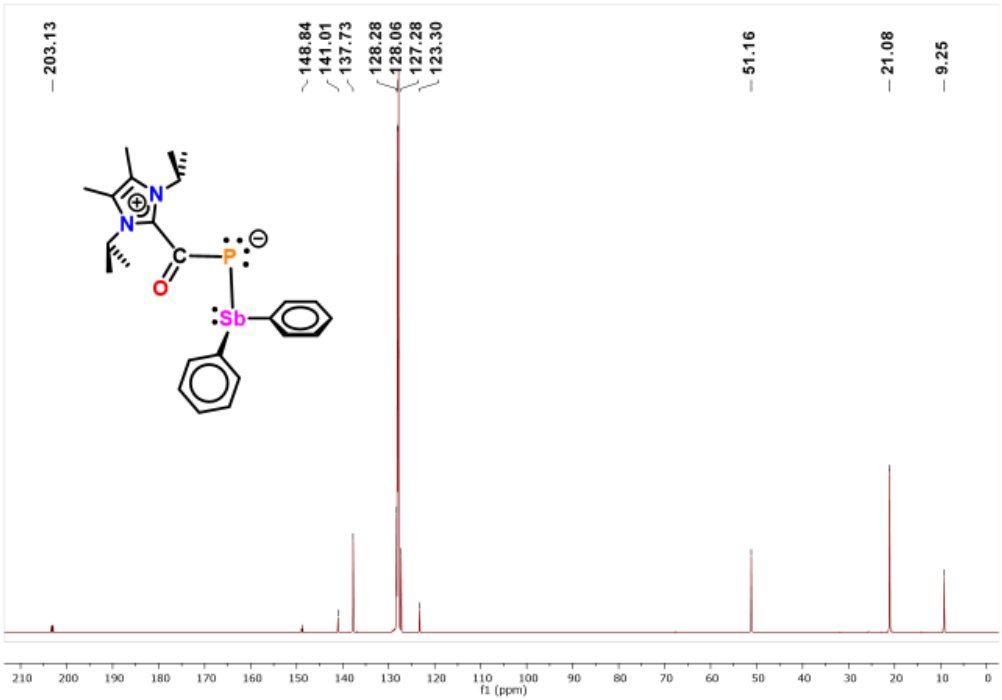


Figure S6: ^{13}C{^{1}H} NMR spectrum (201.193 MHz, C_6D_6, 298 K) of complex **3**.

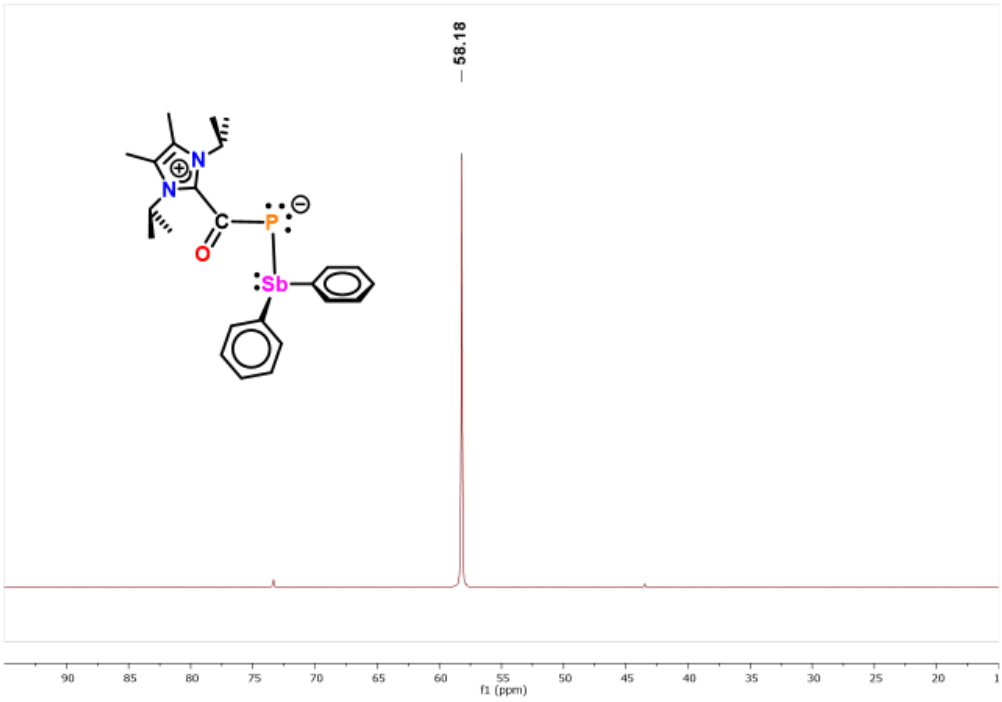


Figure S7: $^{31}P\{^{1}H\}$ NMR spectrum (202.46 MHz, 298 K) of complex **3**.

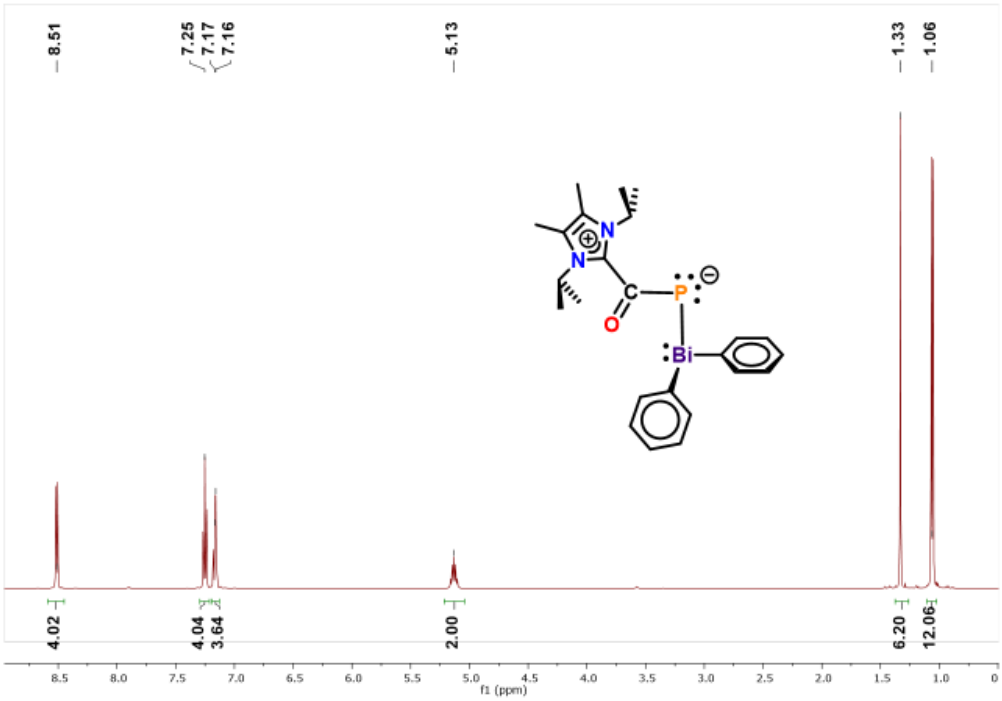


Figure S8: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of complex **4**.

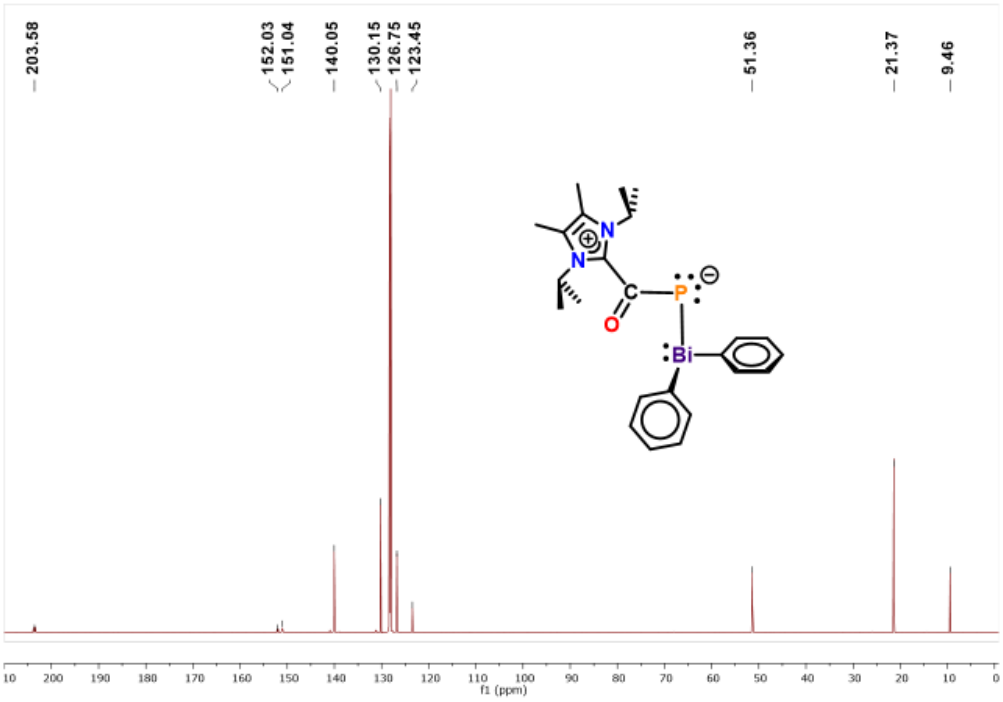


Figure S9: $^{13}C\{^{1}H\}$ NMR spectrum (201.193 MHz, C_6D_6, 298 K) of complex **4**.

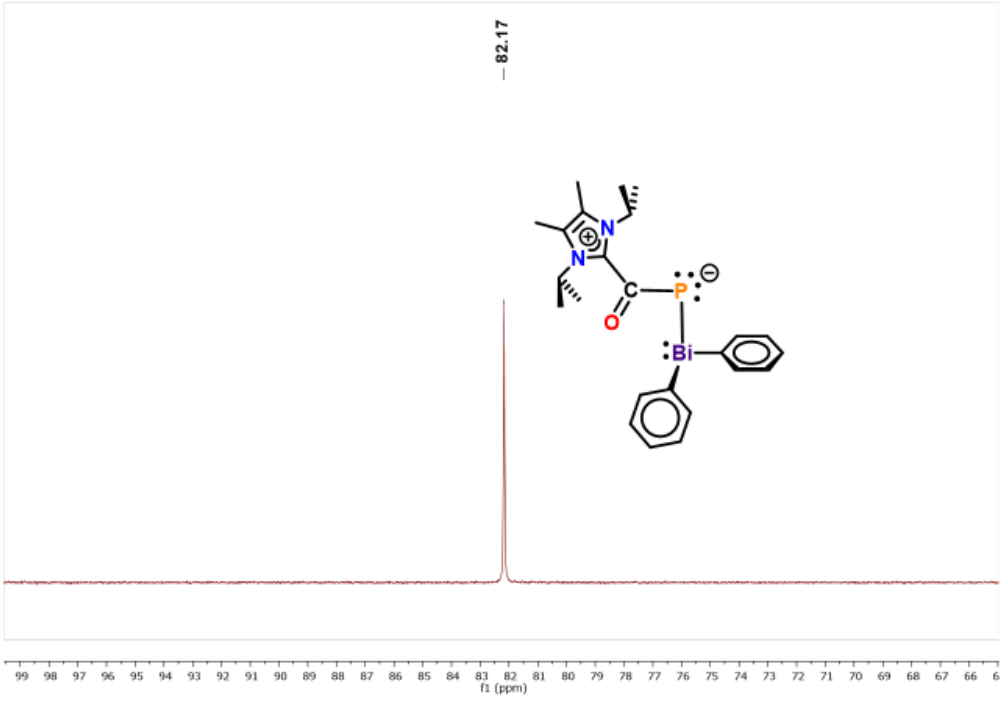


Figure S10: $^{31}P\{^{1}H\}$ NMR spectrum (202.46 MHz, 298 K) of complex **4**.

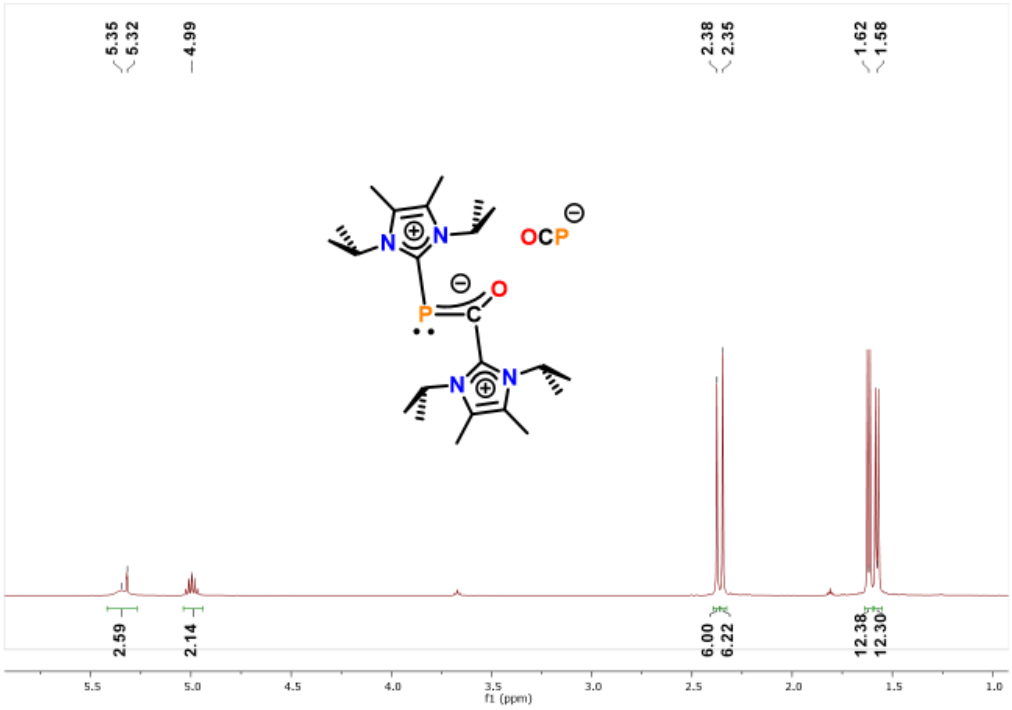


Figure S11: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of complex **5**.

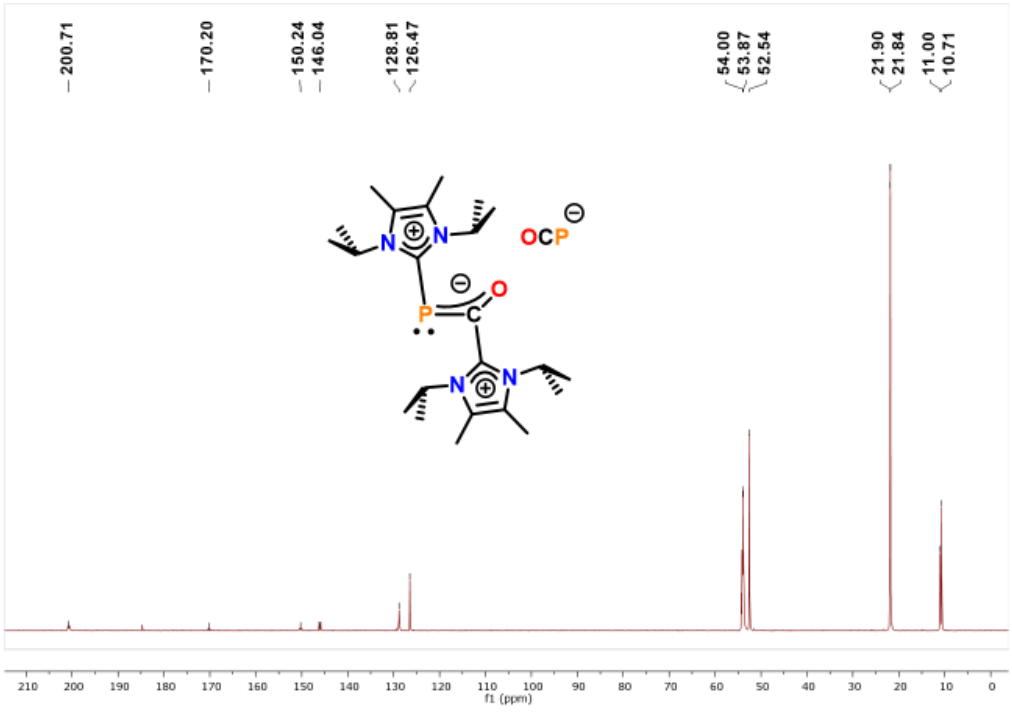


Figure S12: $^{13}C\{^{1}H\}$ NMR spectrum (201.193 MHz, C_6D_6, 298 K) of complex **5**.

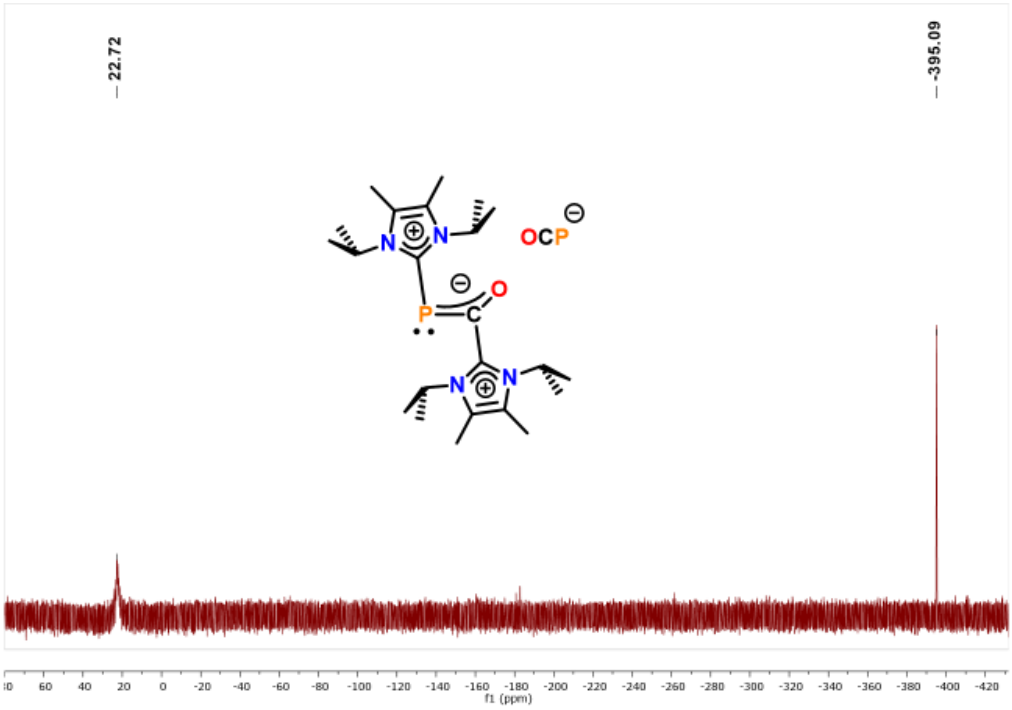


Figure S13: $^{31}P\{^{1}H\}$ NMR spectrum (242.94 MHz, 298 K) of complex **5**.

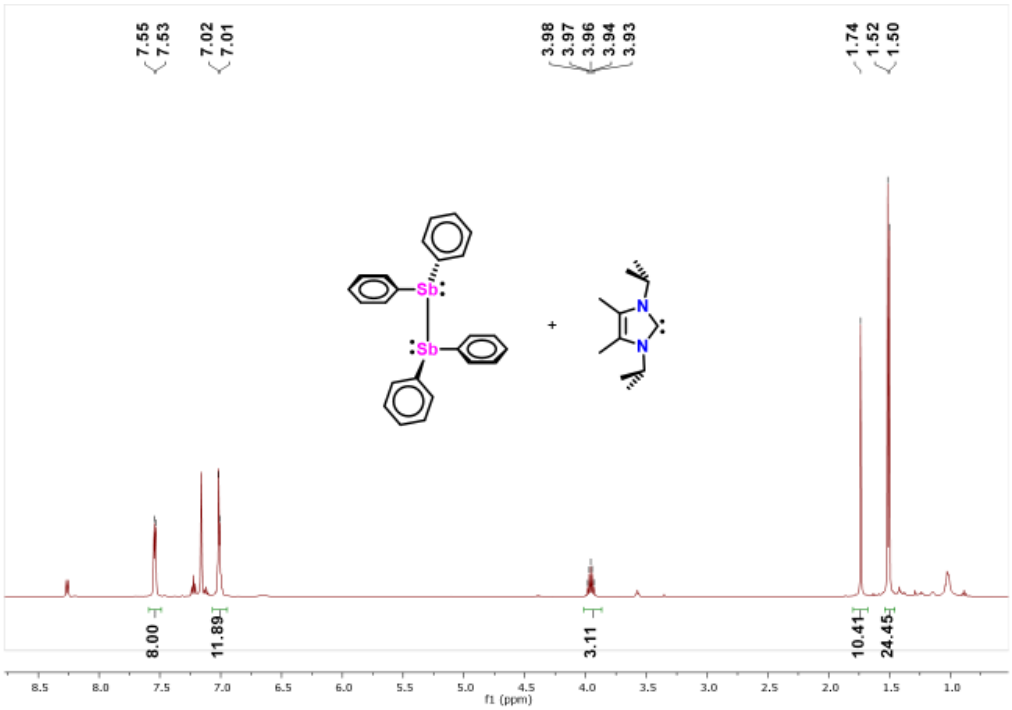


Figure S14: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of the reaction mixture after heating compound **3** at 90 °C for 24 hours.

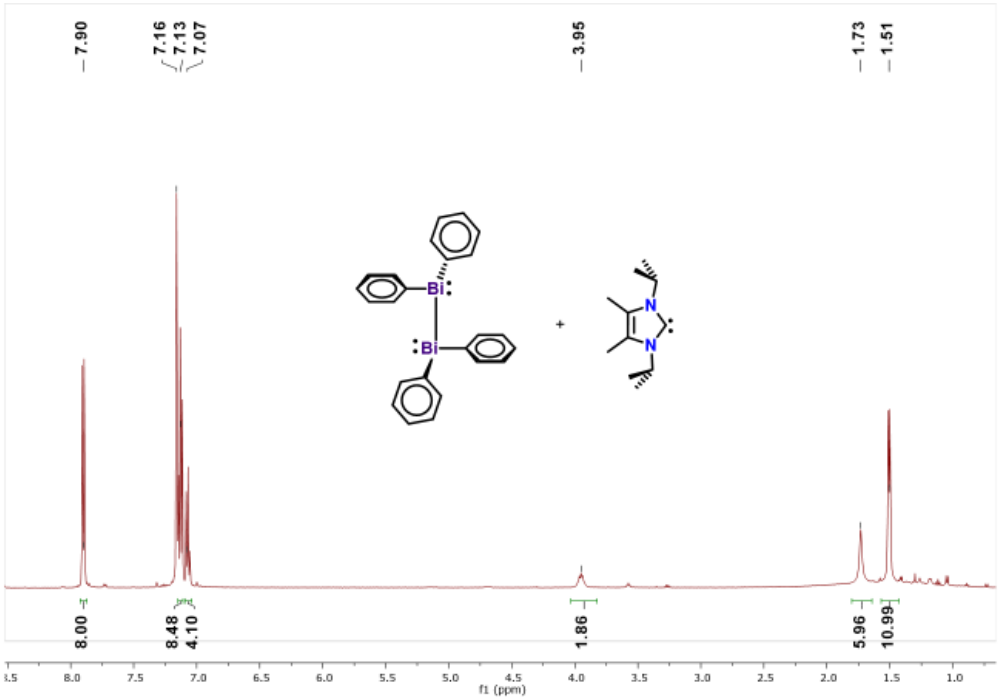


Figure S15: ^{1}H NMR spectrum (500.13 MHz, C_6D_6, 298 K) of the reaction mixture after heating compound **4** at 70 °C for 3 hours.

IR Spectral Data

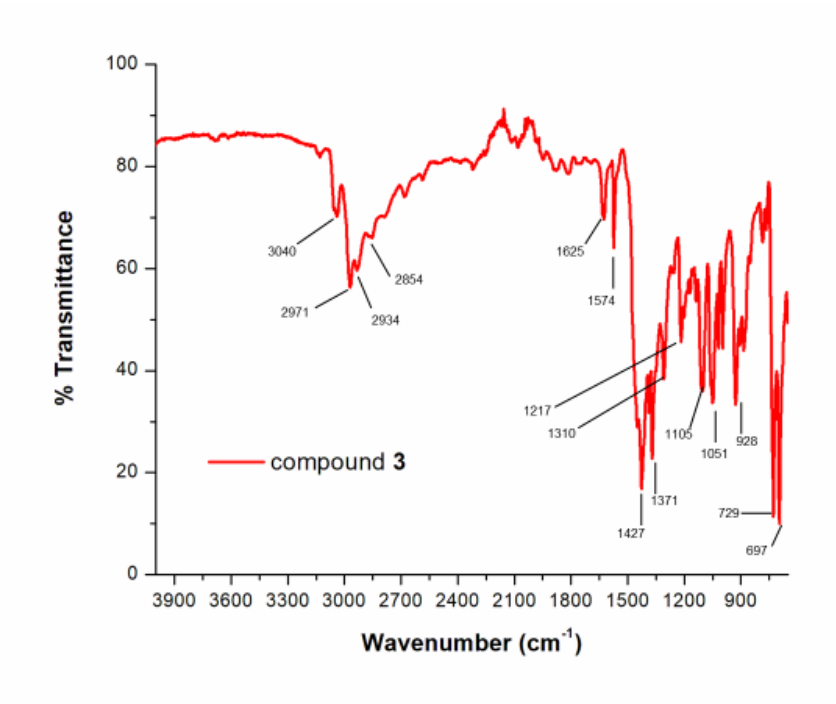


Figure S16: FT-IR Spectrum of compound **3**.

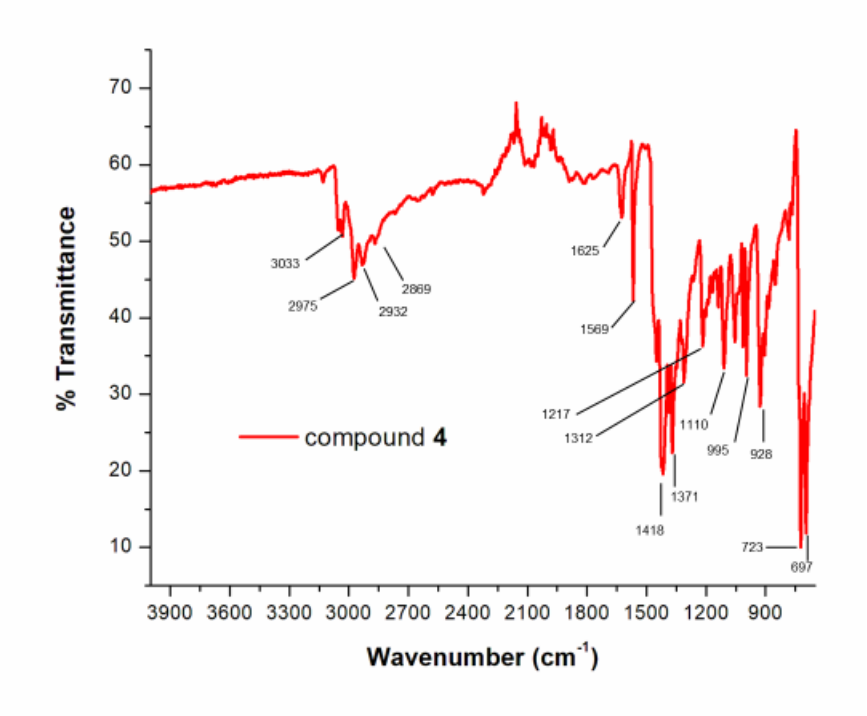


Figure S17: FT-IR Spectrum of compound **4**.

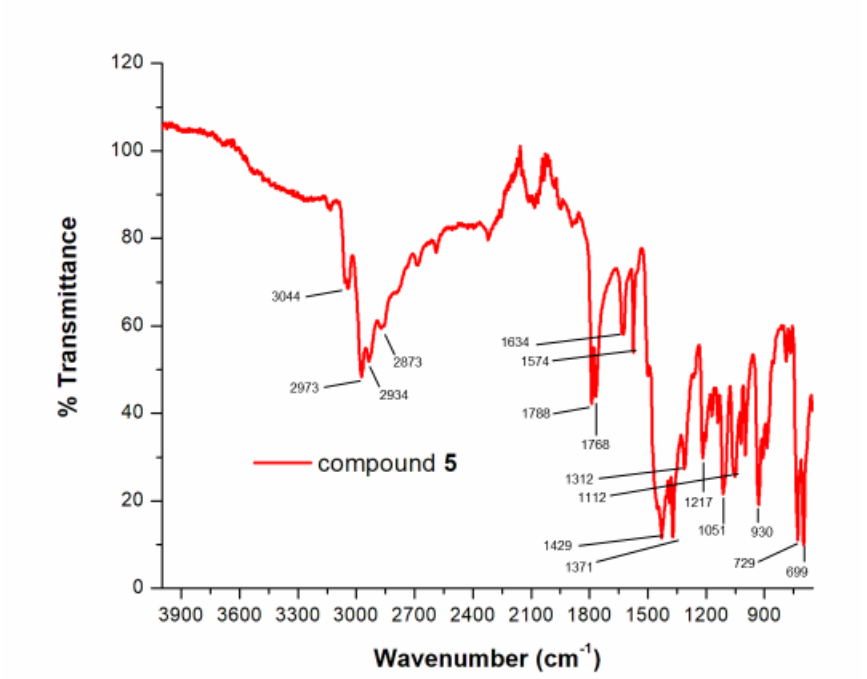


Figure S18: FT-IR Spectrum of compound **5**.

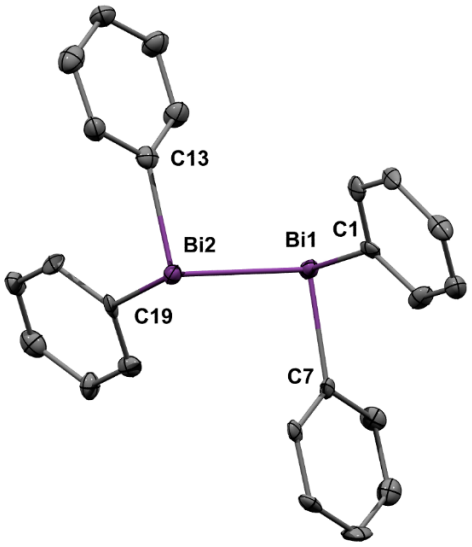


Figure S19: X-ray crystal structure of **6**. Ellipsoids represent 50% probability and all hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Bi1–Bi2: 2.9867(7); Bi1–C1: 2.274(13); Bi1–C7: 2.267(12); Bi2–C13: 2.261(13); Bi2–C19: 2.261(12). C1–Bi1–Bi2: 90.5(3); C7–Bi1–Bi2: 94.0(3); C7–Bi1–C1: 92.3(4); Bi1–Bi2–C13: 95.0(3); Bi1–Bi2–C19: 91.9(3); C13–Bi2–C19: 93.0(5).

Crystallographic Refinement Details

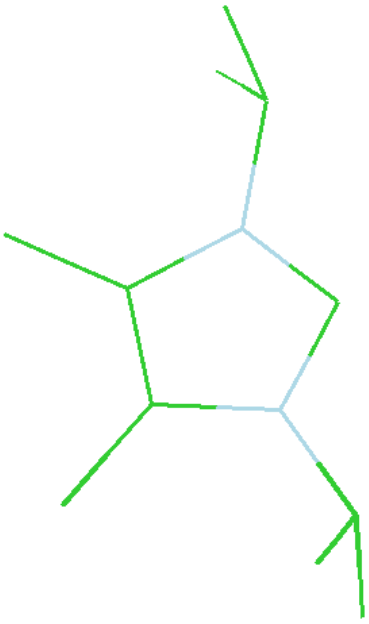
Table S1. Crystallographic data for **1-6**.

	1	**2**	**3**	**4**	**5**	**6**
CCDC	1962839	1962840	1962841	1962842	1976639	1962843
Chemical formula	$C_{23}H_{30}ClN_2Sb$	$C_{23}H_{30}BiClN_2$	$C_{24}H_{30}N_2OPSb$	$C_{24}H_{30}BiN_2OP$	$C_{24}H_{38}N_4O_2P_2$	$C_{24}H_{20}Bi_2$
FW (g/mol)	491.69	578.92	515.22	602.45	476.52	726.36
T (K)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
λ (Å)	1.54178	0.71073	1.54178	1.54178	0.71073	0.71073
Crystal size (mm)	0.063 × 0.086 × 0.134	0.075 × 0.093 × 0.125	0.027 × 0.033 × 0.179	0.046 × 0.049 × 0.088	0.168 × 0.314 × 0.379	0.066 × 0.087 × 0.305
Crystal habit	colorless plate	colorless rod	yellow rod	yellow rod	orange block	yellow rod
Crystal system	triclinic	triclinic	triclinic	monoclinic	orthorhombic	monoclinic
Space group	P -1	P -1	P -1	P $2_1/c$	F dd2	$P2_1$
a (Å)	9.9641(14)	9.9533(12)	11.3208(7)	11.2834(3)	17.553(2)	5.9018(6)
b (Å)	10.2681(16)	10.1962(12)	13.4788(9)	18.2355(5)	22.829(2)	21.746(2)
c (Å)	10.9350(14)	11.0990(14)	17.8244(12)	23.2146(6)	13.3554(15)	16.0512(16)
α (°)	90.719(10)	91.596(4)	92.540(4)	90	90	90
β (°)	96.231(9)	95.821(4)	108.009(4)	95.508(2)	90	92.145(3)
γ (°)	93.539(11)	93.214(4)	111.776(4)	90	90	90
V (Å^3)	1109.8(3)	1118.2(2)	2362.8(3)	4754.5(2)	5351.7(10)	2058.5(4)
Z	2	2	4	8	8	4
ρ_{calc} (g/cm$^{3)}$	1.471	1.719	1.448	1.683	1.183	2.344
μ (mm^{-1})	11.024	8.013	10.023	15.313	0.189	17.078
F(000)	500	564	1048	2352	2048	1320
θ range (°)	4.07 - 68.38°	3.69 - 51.48	2.65 - 68.53	3.09 - 68.39	2.11 to 25.35	2.53 - 56.70
Index ranges	$-11 \le h \le 11$ $-12 \le k \le 12$ $-13 \le l \le 12$	$-12 \le h \le 12$ $-12 \le k \le 12$ $-13 \le l \le 11$	$-13 \le h \le 13$ $-16 \le k \le 16$ $-19 \le l \le 21$	$-10 \le h \le 13$ $-21 \le k \le 21$ $-27 \le l \le 27$	$-20 \le h \le 21$ $-27 \le k \le 26$ $-15 \le l \le 16$	$-7 \le h \le 7$ $-28 \le k \le 28$ $-21 \le l \le 21$
Reflns coll.	14729	18501	34781	37832	10231	36083
Ind. reflns	4033 [R_{int} = 0.0593]	4264 [R_{int} = 0.0725]	8638 [R_{int} = 0.0681]	8710 [R_{int} = 0.0899]	2390 [R(int) = 0.0350]	10223 [R_{int} = 0.0667]
Data / restraints / parameters	4033 / 0 / 250	4264/0/250	8638 / 0 / 550	8710 / 0 / 559	2390 / 23 / 218	10223/1/469
Goodness-of-fit on F^2	1.053	1.034	1.057	1.012	1.079	1.009
R_1 [I>2σ(I)]	0.0338	0.0370	0.0604	0.0411	0.0519	0.0364
wR_2 [all data]	0.0875	0.0673	0.1643	0.0957	0.1414	0.0705

Computational Details

The computations were carried out with the Gaussian 09 suite of programs.[1] The structures were optimized using the ωB97XD functionals. We applied the def2-SVP basis set and we validated the calculations with def2-TZVP basis set implemented in Gaussian 09. At each of the optimized structures vibrational analysis was accomplished to check whether the stationary point located is a minimum or a saddle point of the potential energy hypersurface. We neglected the solvent-effect, because toluene was used as solvent, so the gas-phase computations simulated the reaction-conditions well. For Wiberg Bond Indexes and NPA charges the NBO program version 3.1 was employed.[2] The plotting of the orbitals was carried out with the AVOGADRO program (www.avogadro.cc).

Figure S20. Chemical structure of NHC-carbene with Cartesian X,Y,Z-coordinates (ωb97xd def2-TZVP).



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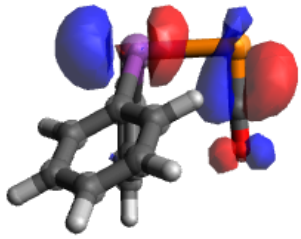
C	0.004640	-0.001670	0.004960
C	0.004648	0.002192	1.359943
N	1.342368	0.002239	1.744223
C	2.183472	-0.008090	0.682455
N	1.342313	-0.011877	-0.379312
C	-1.160982	0.028810	2.287777
C	1.890975	-0.055945	3.098484
C	1.406931	1.080295	3.991267
C	1.891290	0.042113	-1.733590
C	1.398154	-1.090207	-2.626367
C	-1.161127	-0.019517	-0.922910
C	1.691918	-1.428165	3.731768
C	1.702969	1.415902	-2.366757
H	2.958374	0.081466	2.927466
H	2.957591	-0.103706	-1.562678
H	-2.078915	0.180943	-0.372385
H	-1.079079	0.740598	-1.700236
H	-1.276183	-0.986920	-1.415938
H	-1.268784	0.997054	2.780785
H	-2.080230	-0.164760	1.737223
H	-1.084669	-0.731895	3.065111
H	2.012469	-1.132842	-3.527101
H	1.478231	-2.049061	-2.113131
H	0.364558	-0.948352	-2.942937
H	2.239471	1.464008	-3.315966
H	0.652862	1.633145	-2.568407
H	2.095505	2.190177	-1.707357

H	2.228094	-1.480410	4.680943
H	0.640148	-1.637128	3.933509
H	2.078310	-2.205549	3.072397
H	2.021857	1.118265	4.891794
H	1.494305	2.038435	3.477886
H	0.372383	0.946542	4.308227

Figure S21. Chemical structure of $BiPh_2PCO$ with Cartesian X,Y,Z-coordinates (ωb97xd def2-TZVP with contour value 0,05).



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C	2.489362	-0.225693	1.442317
C	2.574975	-0.073909	0.067404
C	1.417052	0.056237	-0.684472
Bi	-1.966500	-0.214018	2.227461
C	-2.585568	1.815068	1.510055
C	-3.942077	2.128220	1.547999
C	-4.394364	3.361651	1.102892
C	-3.491346	4.292874	0.612711
C	-2.139272	3.989494	0.572876
C	-1.686702	2.756536	1.020318

P	-1.345979	0.381058	4.741081
H	-4.663535	1.412952	1.930364
H	-5.451233	3.595142	1.139115
H	-3.840973	5.256332	0.263527
H	-1.430604	4.716165	0.195225
H	-0.626336	2.538060	0.988784
H	1.199208	-0.355511	3.144630
H	3.390247	-0.324123	2.035175
H	3.542460	-0.052996	-0.418274
H	1.477160	0.178728	-1.758832
H	-0.713710	0.151040	-0.665901
C	-0.613785	1.767891	4.205453
O	-0.086683	2.742549	3.887146

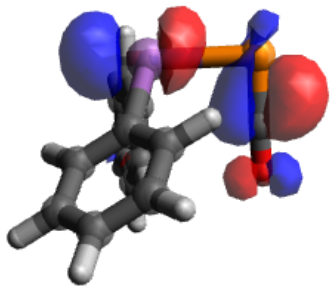
Table S2. Bond length and Wiberg-bond index of characteristic bonds.

Bond	Bond lengths (Å)	Wiberg-bond index
Bi-P	2,657	0,76
P-C	1,657	1,72
C-O	1,153	1,93

Table S3. Natural charges of main atoms.

Atom	Charge
Bi	+1,01
P	-0,14
C	+0,31
O	-0,47

Figure S22. Chemical structure of $SbPh_2PCO$ with Cartesian X,Y,Z-coordinates (ωb97xd def2-TZVP with contour value 0,05).



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C	0.193646	0.238025	-0.004771
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C	1.233279	-0.352294	2.073471
C	2.467765	-0.397376	1.441994
C	2.567406	-0.121877	0.087293
C	1.427954	0.196457	-0.635619
Sb	-1.871697	-0.082962	2.249146
C	-2.548762	1.818484	1.519423
C	-3.925804	2.028303	1.483993
C	-4.447589	3.228215	1.025439
C	-3.595026	4.231699	0.591901
C	-2.223014	4.032668	0.621781
C	-1.701207	2.833112	1.082503

P	-1.299823	0.503007	4.675085
H	-4.606698	1.251802	1.816903
H	-5.519928	3.376755	1.003091
H	-3.999388	5.168941	0.230606
H	-1.553647	4.815149	0.286603
H	-0.627220	2.694879	1.099557
H	1.173738	-0.561292	3.135514
H	3.353614	-0.646825	2.012596
H	3.531622	-0.152443	-0.404294
H	1.498569	0.415679	-1.693793
H	-0.684492	0.496566	-0.586690
C	-0.452451	1.828004	4.143145
O	0.149280	2.756460	3.823278

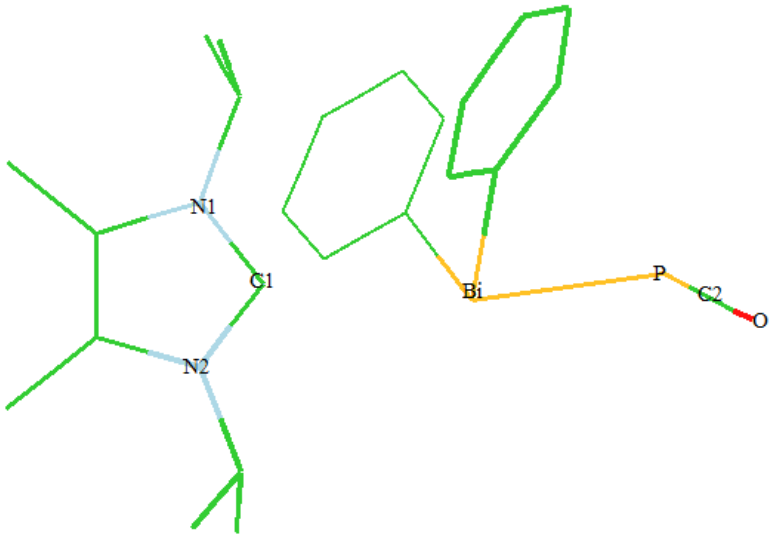
Table S4. Bond length and Wiberg-bond index of characteristic bonds.

Bond	Bond lengths (Å)	Wiberg-bond index
Sb-P	2,551	0,79
P-C	1,662	1,70
C-O	1,152	1,94

Table S5. Natural charges of main atoms.

Atom	Charge
Sb	+0,97
P	-0,13
C	+0,32
O	-0,46

Figure S23. Chemical structure of NHC-BiPh_2PCO complex with carthesian X,Y,Z-coordinates (ωb97xd def2-TZVP).



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N	2.182473	0.937557	-0.565611
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C	3.825456	-0.520790	-0.507149
C	3.563509	0.809505	-0.521955
C	2.326610	-2.599586	-0.542490
C	2.553637	-3.211636	0.833441
C	5.149227	-1.203330	-0.474701
C	4.528514	1.942728	-0.472558
C	1.403970	2.179281	-0.676816
C	1.521830	2.784536	-2.069252
C	3.060196	-3.343054	-1.651566
C	1.702773	3.177986	0.431593
Bi	-1.020488	-0.897046	0.264061
P	-3.513234	-0.890805	1.504627

C	-4.108282	-1.534845	0.115626
O	-4.548537	-1.987687	-0.859959
C	-1.663234	0.519447	-1.371505
C	-1.066932	0.381312	-2.621475
C	-1.446876	1.187232	-3.684817
C	-2.423988	2.154316	-3.506657
C	-3.030146	2.295177	-2.268039
C	-2.660921	1.473747	-1.211393
C	-0.381183	0.575578	1.853997
C	0.767682	0.285553	2.583768
C	1.187883	1.112894	3.615805
C	0.464577	2.254704	3.925131
C	-0.677769	2.558576	3.200464
C	-1.099793	1.720612	2.177121
H	0.376798	1.847465	-0.550920
H	1.261274	-2.664819	-0.760852
H	5.925344	-0.487060	-0.211944
H	5.182285	-2.000431	0.267596
H	5.410112	-1.636354	-1.441907
H	4.514355	2.439995	0.498514
H	5.538922	1.577927	-0.647522
H	4.316550	2.692776	-1.233566
H	2.619365	-4.333835	-1.767100
H	2.963441	-2.816261	-2.601407
H	4.118586	-3.479430	-1.432786
H	2.273041	-4.265586	0.819258
H	3.597537	-3.146764	1.142242

H	1.942206	-2.708150	1.583087
H	0.791553	3.587797	-2.174809
H	2.512078	3.203817	-2.254457
H	1.306833	2.035725	-2.830519
H	0.911638	3.927886	0.448312
H	1.717884	2.687788	1.404351
H	2.647648	3.699107	0.277817
H	-3.181002	1.563511	-0.265084
H	-3.805417	3.038110	-2.124919
H	-2.720171	2.788740	-4.332846
H	-0.976554	1.060912	-4.652668
H	-0.282396	-0.352341	-2.771727
H	-2.006764	1.967137	1.638443
H	-1.248676	3.448415	3.436446
H	0.789351	2.905241	4.727535
H	2.081882	0.866180	4.175838
H	1.359671	-0.592805	2.347929

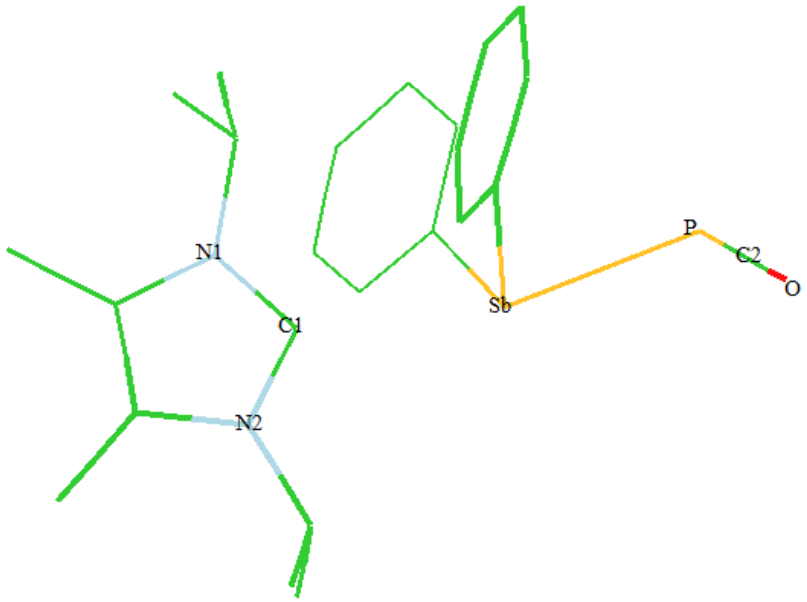
Table S6. Bond length and Wiberg-bond index of characteristic bonds.

Bond	Bond lengths (Å)	Wiberg-bond index
N1-C1	1,348	1,28
N2-C1	1,350	1,27
C1-Bi	2,801	0,26
C2-O	1,162	1,86
P-C2	1,643	1,84
Bi-P	2,784	0,54

Table S7. Natural charges of main atoms.

Atom or unit	Charge
N1	-0,37
N2	-0,38
C1	+0,14
C2	+0,26
O	-0,51
P	-0,23
Bi	+1,12
Carbene	+0,19

Figure S24. Chemical structure of NHC-$SbPh_2PCO$ complex with Cartesian X,Y,Z-coordinates (ωb97xd def2-TZVP).



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C	1.535949	2.693747	0.189223
C	0.740867	1.891601	-0.622081
C	-0.331840	2.483595	-1.284227
C	-0.605079	3.836049	-1.142826
C	0.187398	4.619814	-0.317990

C	1.256607	4.043882	0.349880
Sb	1.100449	-0.210428	-1.006004
C	1.482640	-1.077587	0.939322
C	0.850604	-2.285872	1.220658
C	1.080054	-2.952613	2.414737
C	1.936571	-2.406169	3.358288
C	2.573321	-1.204453	3.090088
C	2.359577	-0.554957	1.881974
P	3.701586	0.471619	-1.370352
C	4.060778	-1.128255	-1.278349
O	4.325002	-2.257257	-1.212887
C	-1.381438	-0.352472	-0.122339
N	-1.958837	0.218983	0.952616
C	-3.333702	0.025411	0.946227
C	-3.615656	-0.694810	-0.166681
N	-2.399415	-0.920834	-0.800266
C	-1.161020	0.883293	1.994242
C	-1.577878	2.328460	2.223008
C	-2.172985	-1.628950	-2.065543
C	-2.760180	-3.034710	-2.074137
C	-4.939406	-1.185188	-0.642479
C	-4.283633	0.560359	1.961437
C	-2.605267	-0.792756	-3.262260
C	-1.101793	0.060023	3.273222
H	-0.159474	0.899763	1.577008
H	-1.090292	-1.731035	-2.115000
H	-5.736768	-0.664762	-0.115094

H	-5.086635	-1.004791	-1.706809
H	-5.066694	-2.254485	-0.464708
H	-4.435816	1.634330	1.841272
H	-5.250988	0.072656	1.856656
H	-3.939554	0.384368	2.979098
H	-2.324309	-3.594190	-2.902398
H	-2.523760	-3.559915	-1.147958
H	-3.841051	-3.036237	-2.210427
H	-2.337841	-1.307227	-4.186072
H	-3.681976	-0.618589	-3.275000
H	-2.100450	0.173789	-3.253888
H	-0.379175	0.511099	3.954332
H	-2.062441	0.016919	3.787787
H	-0.769165	-0.954986	3.059133
H	-0.808279	2.825711	2.814041
H	-1.663008	2.858660	1.274650
H	-2.518708	2.411700	2.767283
H	2.906616	0.354998	1.670213
H	3.255508	-0.778443	3.815634
H	2.114352	-2.919191	4.295131
H	0.589026	-3.898540	2.608224
H	0.159870	-2.716385	0.502884
H	2.396329	2.274225	0.695362
H	1.886411	4.649774	0.989675
H	-0.023400	5.675295	-0.200120
H	-1.439625	4.276961	-1.674391
H	-0.974579	1.882445	-1.918752

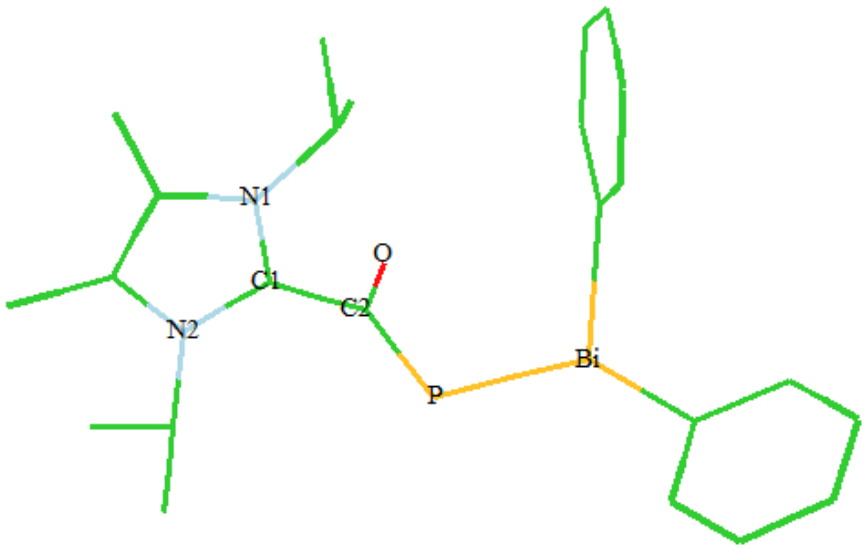
Table S8. Bond length and Wiberg-bond index of characteristic bonds.

Bond	Bond lengths (Å)	Wiberg-bond index
N1-C1	1,347	1,28
N2-C1	1,349	1,27
C1-Sb	2,638	0,32
C2-O	1,161	1,87
P-C2	1,642	1,82
Sb-P	2,714	0,55

Table S9. Natural charges of main atoms.

Atom or unit	Charge
N1	-0,38
N2	-0,37
C1	+0,17
C2	+0,27
O	-0,51
P	-0,23
Sb	+1,06
Carbene	+0,23

Figure S25. Chemical structure of NHC-C(O)PBiPh$_2$ complex with Cartesian X,Y,Z-coordinates (ωb97xd def2-TZVP).



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C	3.260243	-1.908602	1.567785
C	3.383675	-0.921309	0.593476
C	4.527893	-0.125712	0.605012
C	5.515454	-0.303832	1.563709
C	5.377302	-1.291644	2.527371
C	4.247540	-2.094818	2.526444
Bi	1.837473	-0.629560	-1.036163
C	1.577474	1.568592	-0.572297
C	1.154886	2.431517	-1.579249
C	0.942629	3.779490	-1.320617
C	1.146809	4.283264	-0.044934
C	1.562749	3.431276	0.969022
C	1.773253	2.084679	0.706185
P	-0.154796	-1.289772	0.500521
C	-1.247919	-0.483447	-0.592019
O	-1.096070	0.034751	-1.714617
C	-2.620566	-0.261024	0.003036
N	-3.633972	-1.124702	0.063856
C	-4.729520	-0.487726	0.634798
C	-4.346413	0.786917	0.905269
N	-3.024164	0.905784	0.504192
C	-3.506768	-2.519784	-0.397946
C	-4.569823	-2.883832	-1.423973
C	-2.141940	2.093226	0.525178
C	-2.050291	2.720654	1.906315
C	-5.137016	1.880118	1.533299

C	-6.055851	-1.125045	0.857520
C	-2.531173	3.064896	-0.577034
C	-3.433006	-3.481795	0.778014
H	0.972809	2.051935	-2.578310
H	0.614849	4.436897	-2.117471
H	0.987442	5.335699	0.157239
H	1.727831	3.817811	1.968140
H	2.094630	1.430908	1.509070
H	2.378736	-2.540044	1.596650
H	4.129959	-2.865942	3.278624
H	6.145783	-1.432053	3.277648
H	6.393805	0.330808	1.558268
H	4.652865	0.659673	-0.133858
H	-2.537063	-2.538548	-0.894020
H	-1.154423	1.699726	0.287819
H	-6.196467	1.633519	1.505002
H	-4.853479	2.033364	2.575585
H	-5.007014	2.825242	1.008601
H	-5.962802	-2.100798	1.332025
H	-6.658174	-0.499786	1.513221
H	-6.602998	-1.255199	-0.077323
H	-1.809986	3.881456	-0.593000
H	-2.495032	2.562017	-1.543136
H	-3.526064	3.487746	-0.425237
H	-1.217426	3.423526	1.898791
H	-2.949716	3.269629	2.184134
H	-1.842423	1.962655	2.662253

H	-4.278785	-3.814816	-1.910817
H	-5.548479	-3.043525	-0.972601
H	-4.652115	-2.113580	-2.191115
H	-3.226282	-4.485251	0.404504
H	-2.622857	-3.194687	1.448438
H	-4.367673	-3.520265	1.339024

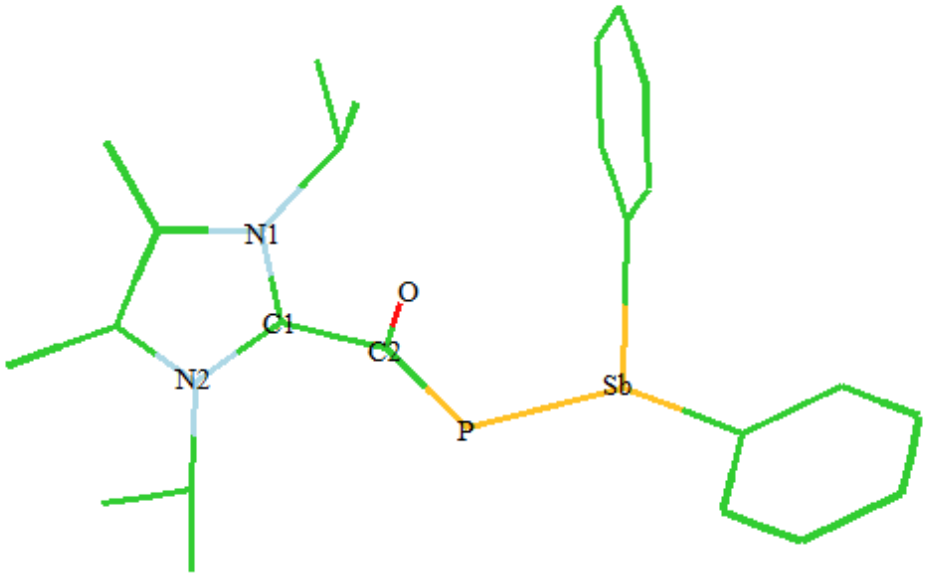
Table S10. Bond length and Wiberg-bond index of characteristic bonds.

Bond	Bond lengths (Å)	Wiberg-bond index
N1-C1	1,332	1,30
N2-C1	1,333	1,30
C1-C2	1,513	0,93
C2-O	1,246	1,47
P-C2	1,743	1,42
Bi-P	2,601	0,91

Table S11. Natural charges of main atoms.

Atom or unit	Charge
N1	-0,29
N2	-0,29
C1	+0,41
C2	+0,04
O	-0,68
P	-0,24
Bi	+0,94
Carbene	+0,75

Figure S26. Chemical structure of NHC-C(O)PSbPh$_2$ complex with Cartesian X,Y,Z-coordinates (ωb97xd def2-TZVP).



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N	-3.410275	-1.123139	-0.019538
C	-2.389142	-0.268841	-0.074650
N	-2.763583	0.880526	0.486062
C	-4.075218	0.759719	0.919726
C	-4.481236	-0.498599	0.608855
C	-1.037944	-0.477313	-0.723585
O	-0.916249	0.090641	-1.823122
C	-1.867377	2.057032	0.529138
C	-2.267412	3.069538	-0.531760
C	-4.834692	1.837447	1.609665
C	-5.806988	-1.131756	0.845933

C	-3.315553	-2.497742	-0.547057
C	-3.214664	-3.512429	0.581548
P	0.081786	-1.340085	0.298699
Sb	2.002378	-0.677720	-1.182969
C	1.829187	1.421599	-0.676097
C	1.420207	2.328060	-1.650123
C	1.239713	3.670719	-1.344189
C	1.466173	4.126233	-0.054356
C	1.872564	3.231893	0.926603
C	2.048525	1.891052	0.617535
C	3.530503	-1.082382	0.298215
C	4.726599	-0.367356	0.248390
C	5.751898	-0.621370	1.146850
C	5.602655	-1.608993	2.109523
C	4.423344	-2.334592	2.166873
C	3.397000	-2.071583	1.269423
C	-4.416951	-2.801068	-1.551850
C	-1.741931	2.638907	1.927519
H	1.223935	1.984044	-2.658882
H	0.919911	4.361346	-2.115461
H	1.331735	5.174551	0.184290
H	2.055857	3.580276	1.936415
H	2.359815	1.202575	1.394640
H	2.477334	-2.641276	1.343131
H	4.297175	-3.105681	2.917525
H	6.401163	-1.810464	2.812949
H	6.670357	-0.049124	1.093764

H	4.862072	0.412503	-0.494188
H	-2.363321	-2.505213	-1.076376
H	-0.889387	1.661136	0.259269
H	-5.895920	1.597190	1.614897
H	-4.510612	1.958600	2.644230
H	-4.718350	2.796537	1.107249
H	-5.709576	-2.127213	1.276760
H	-6.381953	-0.528831	1.545656
H	-6.384695	-1.217033	-0.075505
H	-1.537232	3.878308	-0.535555
H	-2.257597	2.598610	-1.514370
H	-3.253957	3.497928	-0.344646
H	-0.898699	3.329417	1.926587
H	-2.628244	3.191794	2.237871
H	-1.532385	1.855502	2.656662
H	-4.164754	-3.722722	-2.076666
H	-5.385992	-2.949592	-1.076410
H	-4.500986	-2.004216	-2.291138
H	-3.036198	-4.500596	0.156506
H	-2.376977	-3.266105	1.234177
H	-4.129165	-3.563151	1.174084

Table S12. Bond length and Wiberg-bond index of characteristic bonds.

Bond	Bond lengths (Å)	Wiberg-bond index
N1-C1	1,333	1,30
N2-C1	1,333	1,30
C1-C2	1,513	0,93
C2-O	1,244	1,48
P-C2	1,745	1,41
Sb-P	2,515	0,92

Table S13. Natural charges of main atoms.

Atom or unit	Charge
N1	-0,29
N2	-0,29
C1	+0,41
C2	+0,06
O	-0,67
P	-0,24
Sb	+0,90
Carbene	+0,76

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