Electronic Supplementary Material (ESI) for Dalton Transactions.

Avenue to Phosphaalkenes from Ph_3GePCO

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Supplemental Information

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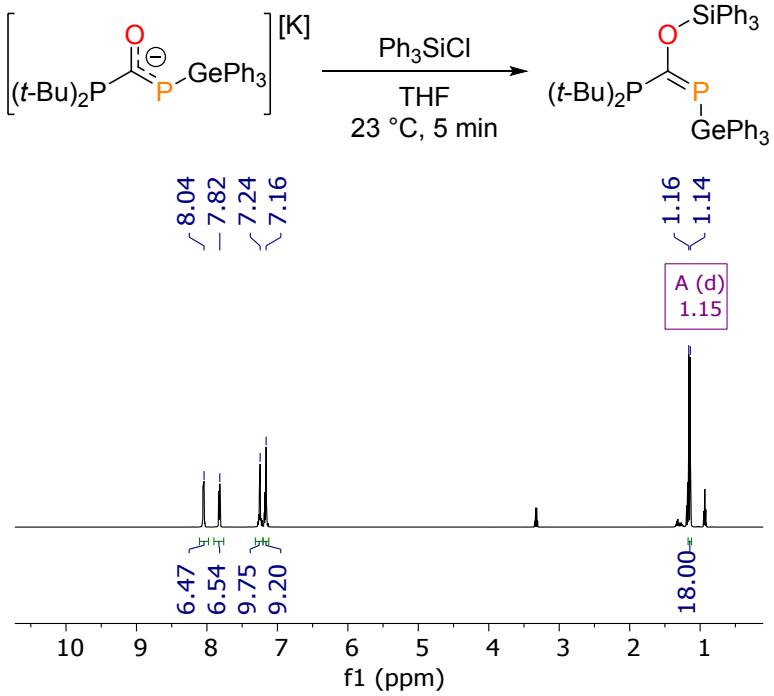


Figure 1. ^{1}H NMR spectrum of (*Z*)-**2** (C_6D_6)

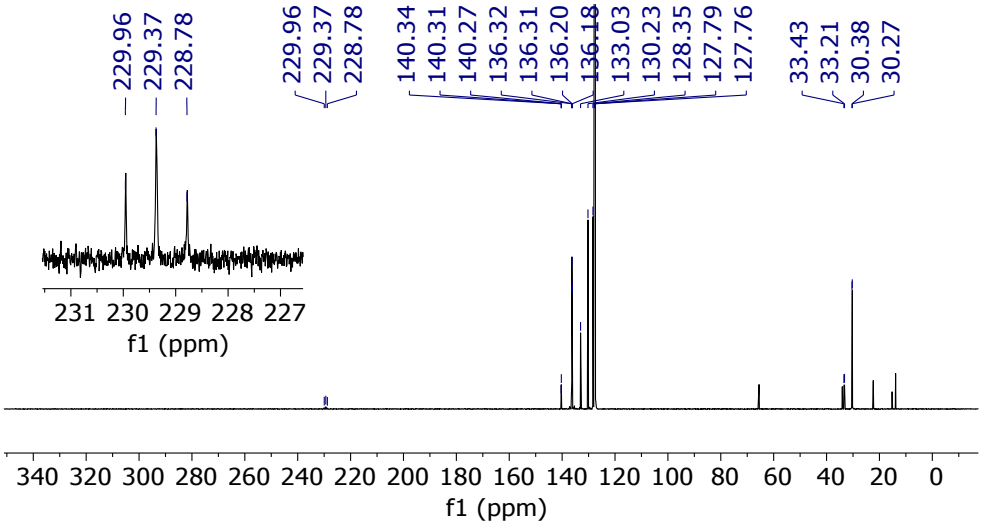


Figure 2. $^{13}C\{^{1}H\}$ NMR spectrum of (*Z*)-**2** (C_6D_6)

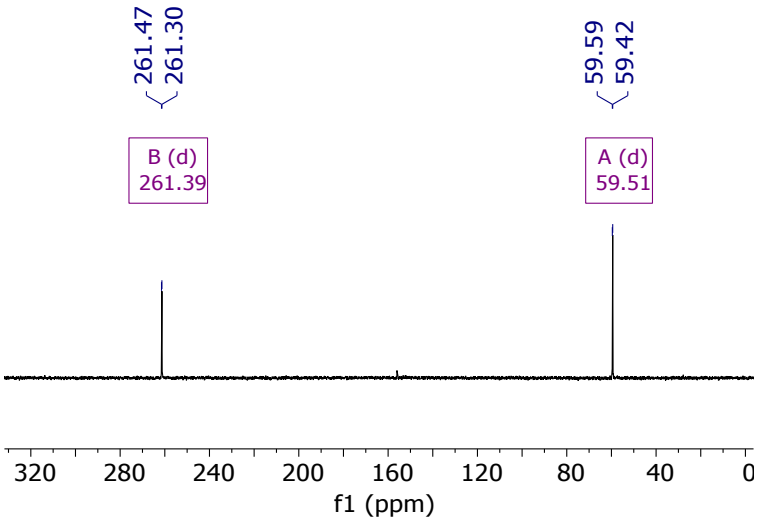


Figure 3. $^{31}P\{^{1}H\}$ NMR spectrum of (*Z*)-**2** (C_6D_6)

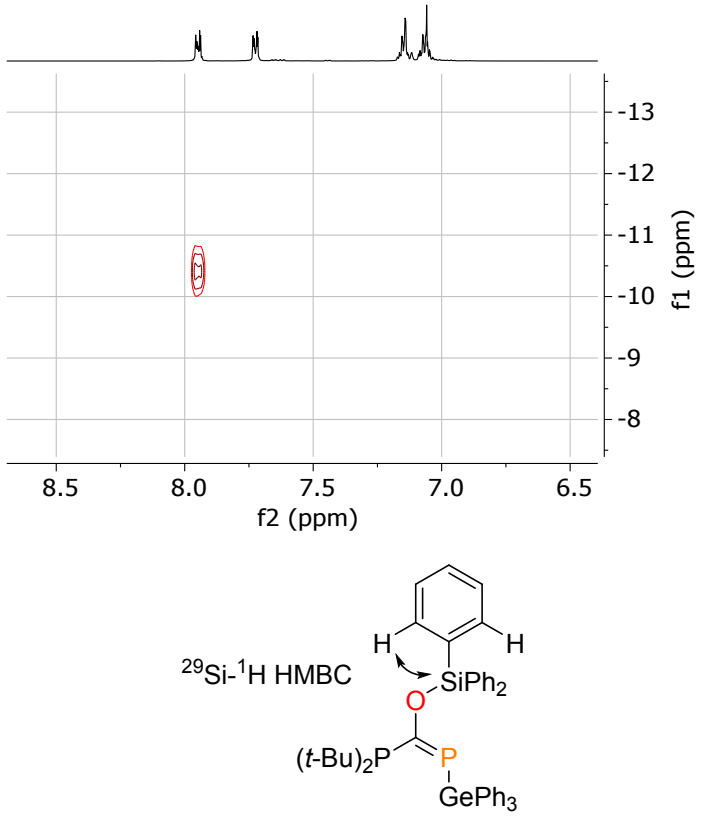


Figure Sx.

Figure 4. ^{29}Si-^{1}H HMBC NMR spectrum of (*Z*)-**2** (C_6D_6)

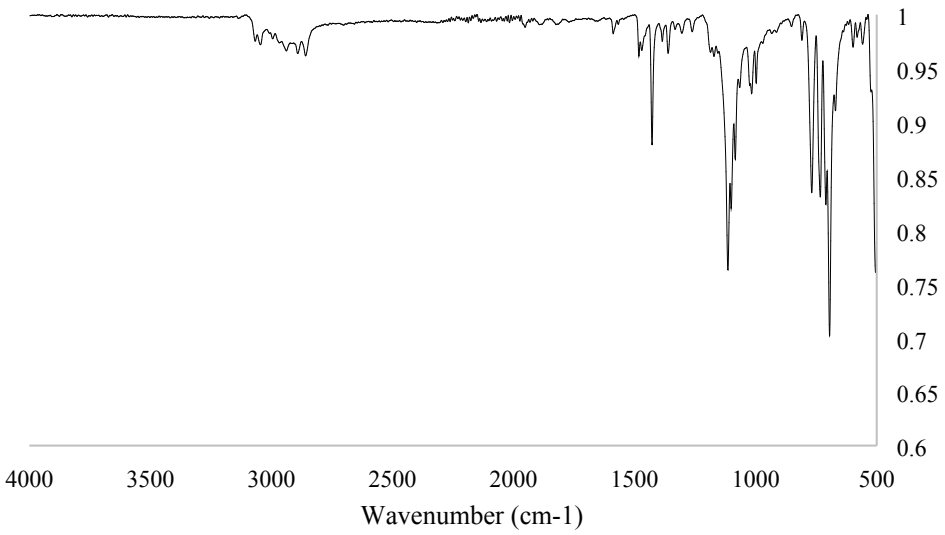
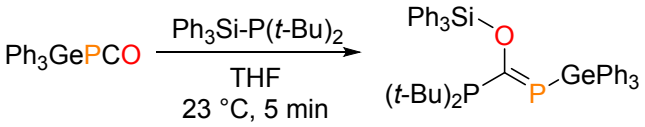


Figure 5. ATR IR spectrum of (*Z*)-**2**

Spectra of (*E*)-**2**



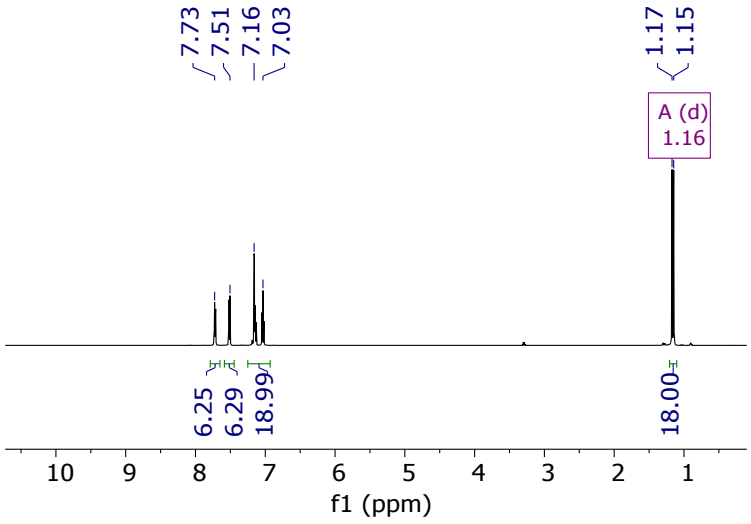


Figure 6. ^{1}H NMR spectrum of (*E*)-**2** (C_6D_6)

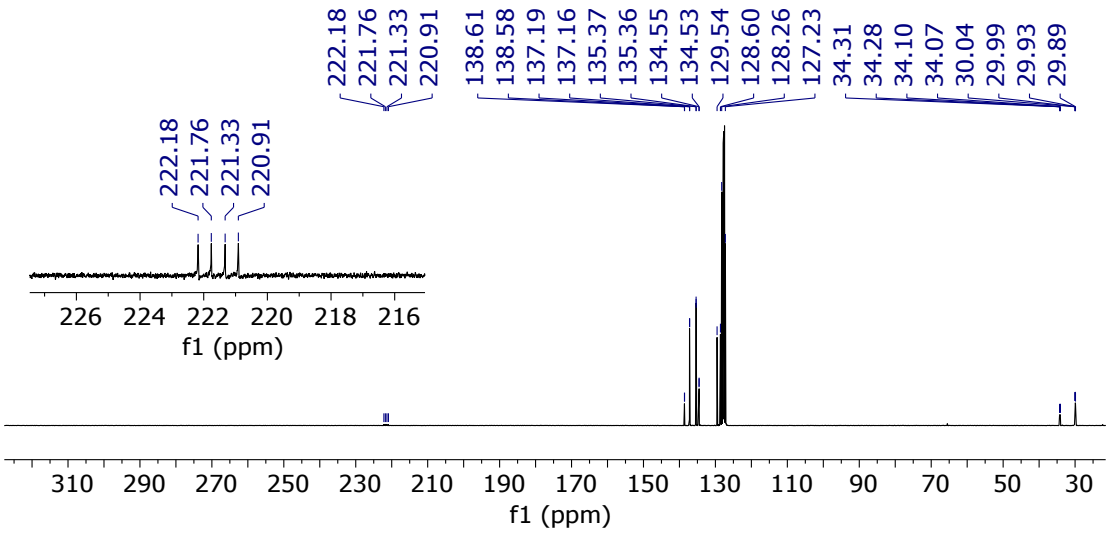


Figure 7. $^{13}C\{^{1}H\}$ NMR spectrum of (*E*)-**2** (C_6D_6)

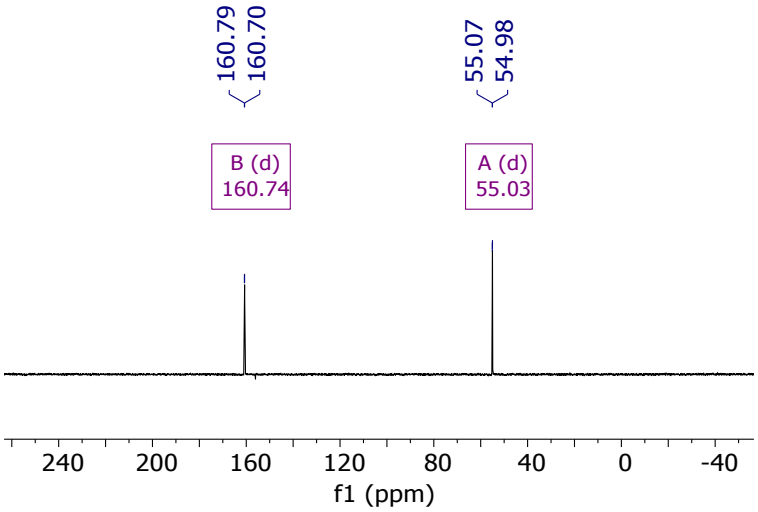


Figure 8. $^{31}P\{^{1}H\}$ NMR spectrum of (*E*)-**2** (C_6D_6)

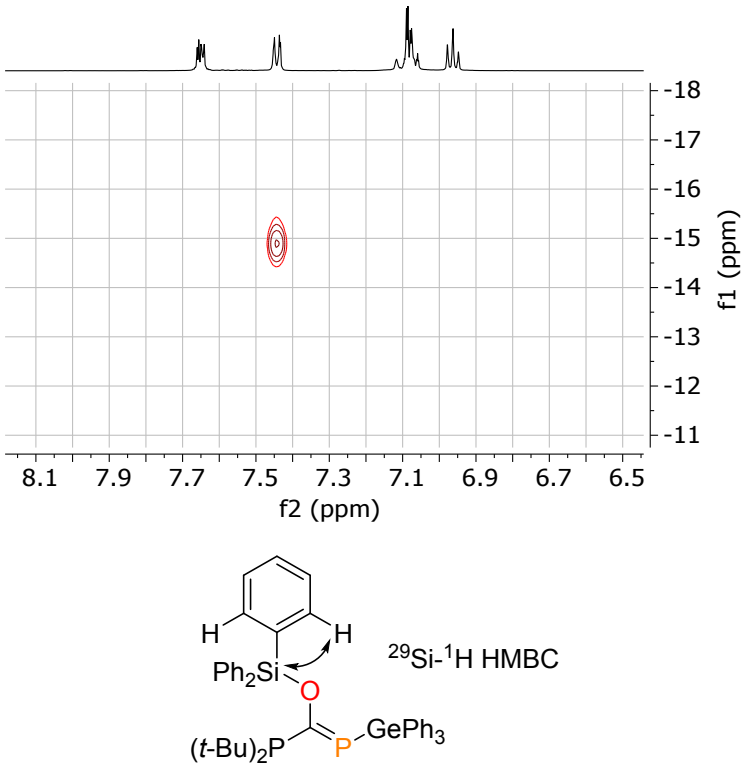


Figure 9. ^{29}Si-^{1}H HMBC NMR spectrum of (*E*)-**2** (C_6D_6)

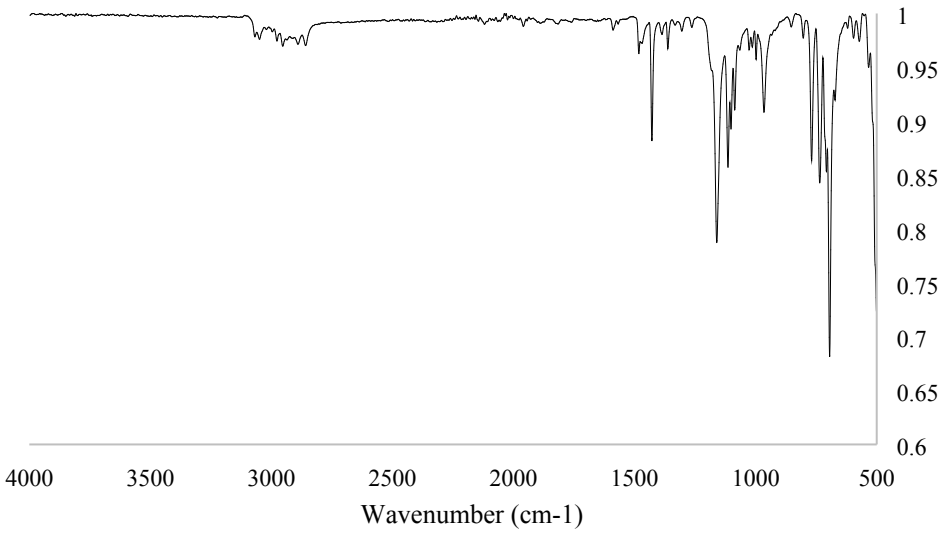


Figure 10. ATR IR spectrum of (*E*)-**2**

Thermal isomerization of (*Z*)-**2** and (*E*)-**2**

In the glovebox, solutions of (*Z*)-**2** and (*E*)-**2** (*ca.* 0.10 M) in tetrahydrofuran were charged into separate NMR tubes. Both solutions were maintained at ambient temperature for 24 hours, then heated in the same oil bath set to 55 °C for a total of 78 hours. The solutions were periodically removed from the oil bath and analyzed by $^{31}P\{^{1}H\}$ NMR spectroscopy.

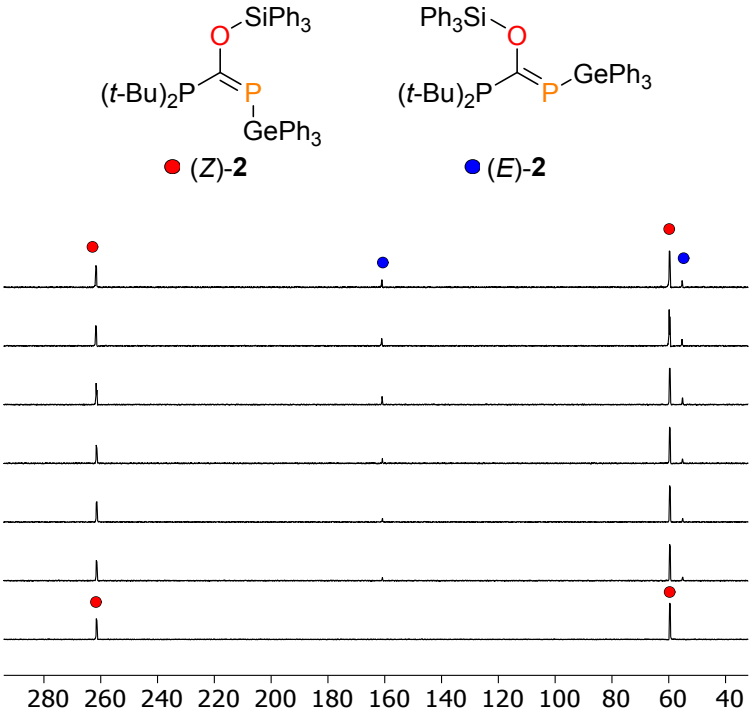


Figure 11. $^{31}P\{^{1}H\}$ NMR spectra of heated solutions of (*Z*)-**2** (THF)

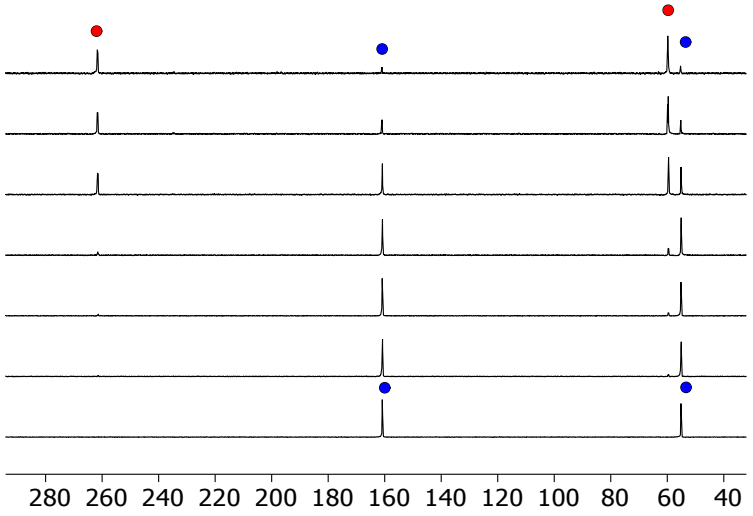


Figure 12. $^{31}P\{^{1}H\}$ NMR spectra of heated solutions of (*E*)-**2** (THF)

Time points (bottom to top): 1 h (23 °C), 24 h (23 °C), 1 h (55 °C), 4.5 h (55 °C), 30 h (55 °C), 55 h (55 °C), 78 h (55 °C)

Photolysis of (*Z*)-**2**

A solution of (*Z*)-**2** (13.8 mg, 0.018 mmol) in C_6D_6 was transferred to a J-Young NMR tube and irradiated for 1 hour. Analysis by $^{31}P\{^1H\}$ NMR spectroscopy revealed isomerization to (*E*)-**2**.

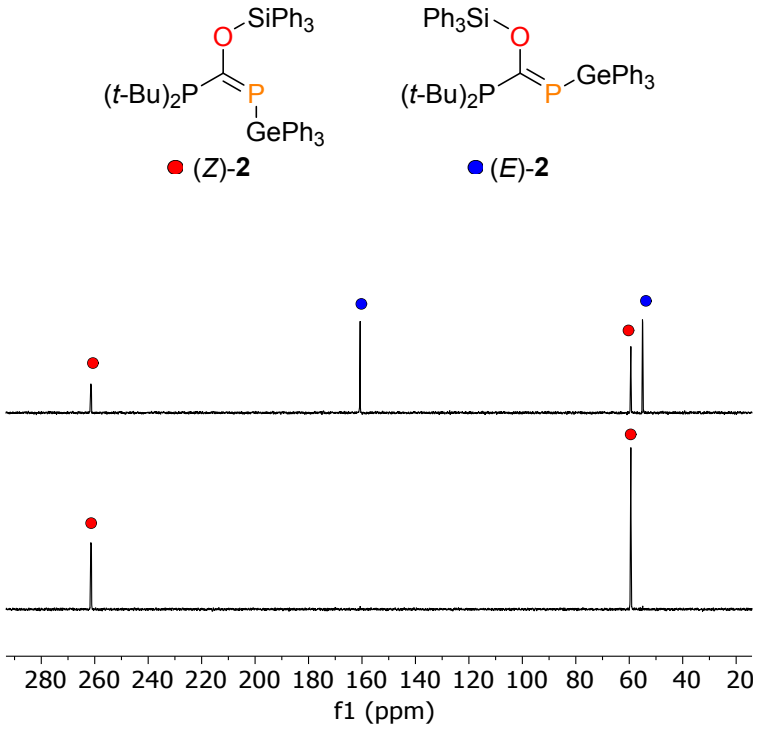


Figure 13. Stacked $^{31}P\{^1H\}$ NMR spectra of photolysis of (*Z*)-**2** (C_6D_6)

Reaction mixture before photolysis (bottom) and after 1 hour of irradiation (top)

Photolysis of (*E*)-**2**

A solution of (*E*)-**2** (18.6 mg, 0.024 mmol) in C_6D_6 was transferred to a J-Young NMR tube and irradiated for 1 hour. Analysis by $^{31}P\{^1H\}$ NMR spectroscopy revealed isomerization to (*Z*)-**2**.

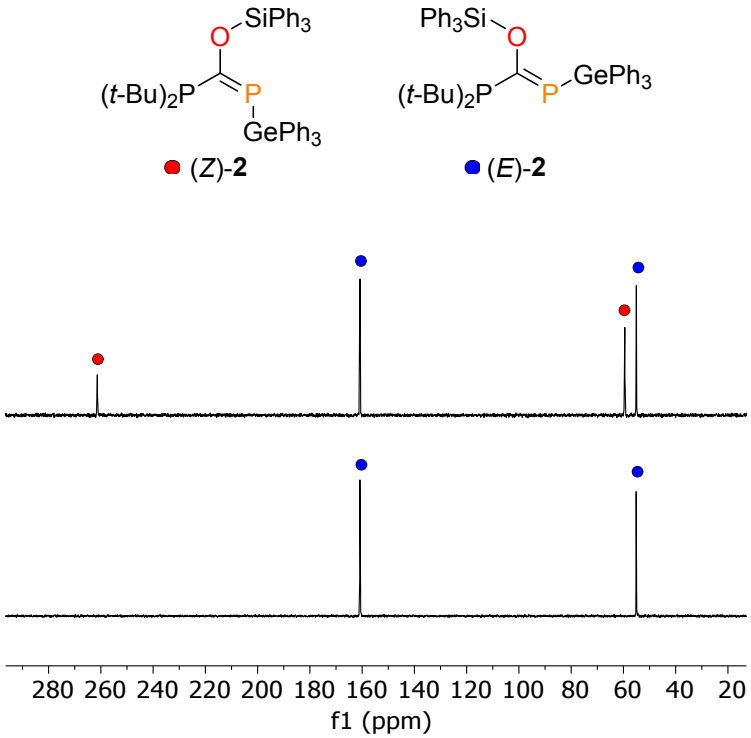
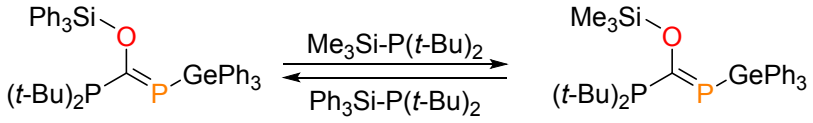


Figure 14. Stacked $^{31}P\{^1H\}$ NMR spectra of photolysis of (*E*)-**2** (C_6D_6)

Reaction mixture before photolysis (bottom) and after 1 hour of irradiation (top)

Reaction of (*E*)-**2** with *t*-Bu_2P-$SiMe_3$



(*E*)-**2** (*E*)-**3**

A solution of (*E*)-**2** (18.3 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL) was combined with a solution of *t*-Bu_2P-$SiMe_3$ (5.2 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL). The homogenous yellow solution was transferred to an NMR tube and analyzed by $^{31}P\{^1H\}$ NMR spectroscopy. Analysis after 30 minutes at ambient temperature shows a small amount of silane exchange as evidenced by the formation of (*E*)-**3**. The lack of signal attrib uted (*Z*)-**2** or (*Z*)-**3** implied that silane exchange occurred without thermal isomerization. Heating the reaction mixture to 85 °C for 1.5 h showed increased silane exchange and the formation of (*Z*)-**2** or (*Z*)-**3**.

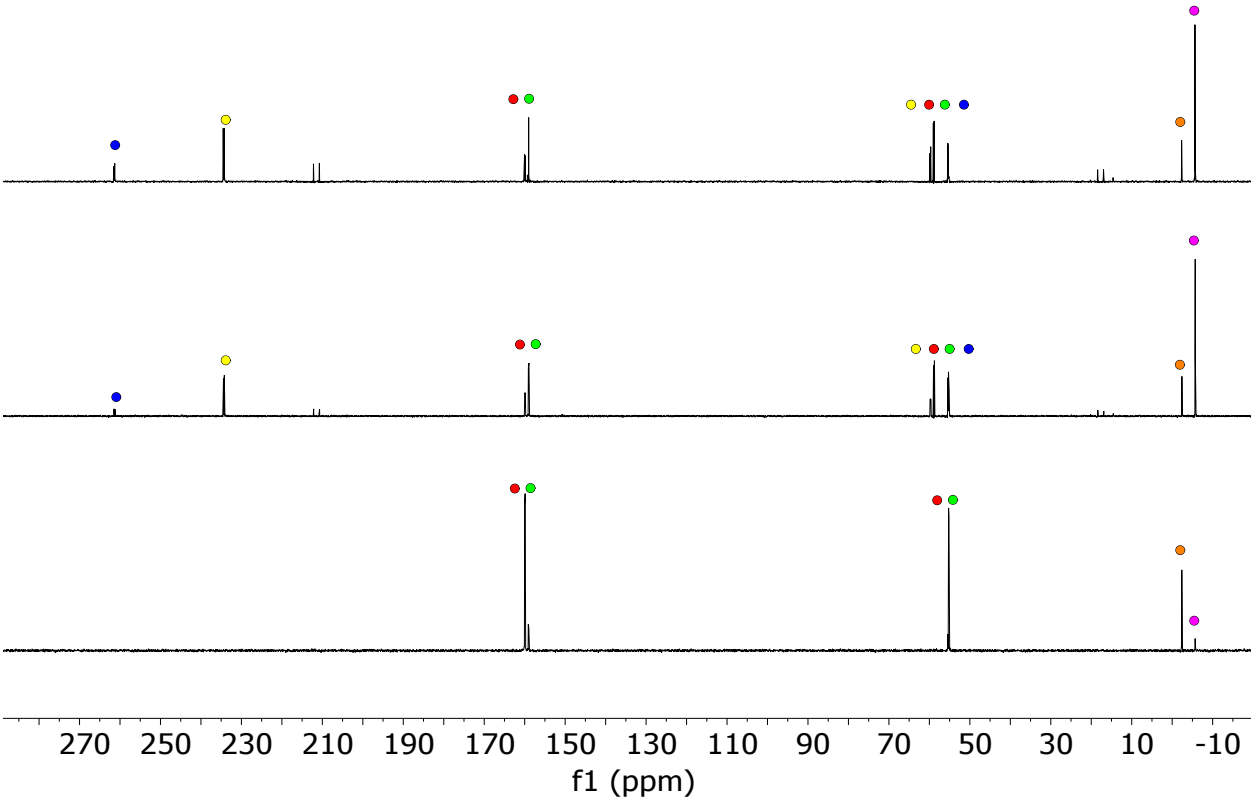
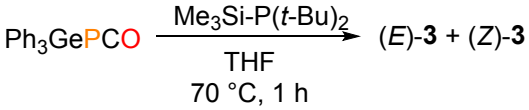


Figure 15. Stacked $^{31}P\{^1H\}$ NMR spectra of displaying silane exchange (THF)

Bottom: 23 °C, 30 min. Middle: 85 °C, 1 h. Top: 85 °C, 2 h.

Ph_3Si-P(*t*-Bu)$_2$ Me_3Si-P(*t*-Bu)$_2$ (*E*)-**2** (*Z*)-**2** (*E*)-**3** (*Z*)-**3**

Independent *in-situ* syntheses and characterization of (*E*)-**3**/(*Z*)-**3**



Equimolar solutions of Ph_3GePCO (20.4 mg, 0.06 mmol, 1 equiv.) and $(t\text{-Bu})_2P\text{-}SiMe_3$ (12.3 mg, 0.06 mmol, 1 equiv.) were combined in tetrahydrofuran (*ca.* 0.6 mL). The pale-yellow reaction mixture was transferred to an NMR tube and analyzed by $^{31}P\{^1H\}$ NMR spectroscopy, which showed complete conversion to (*E*)-**3** (δ 159 ppm, 55 ppm, $^2J_{PP}$ = 20 Hz) and a small amount of (*Z*)-**3** (δ 234 ppm, 59 ppm, $^2J_{PP}$ = 33 Hz). Heating to 70 °C for 1 hour leads to increased isomerization.

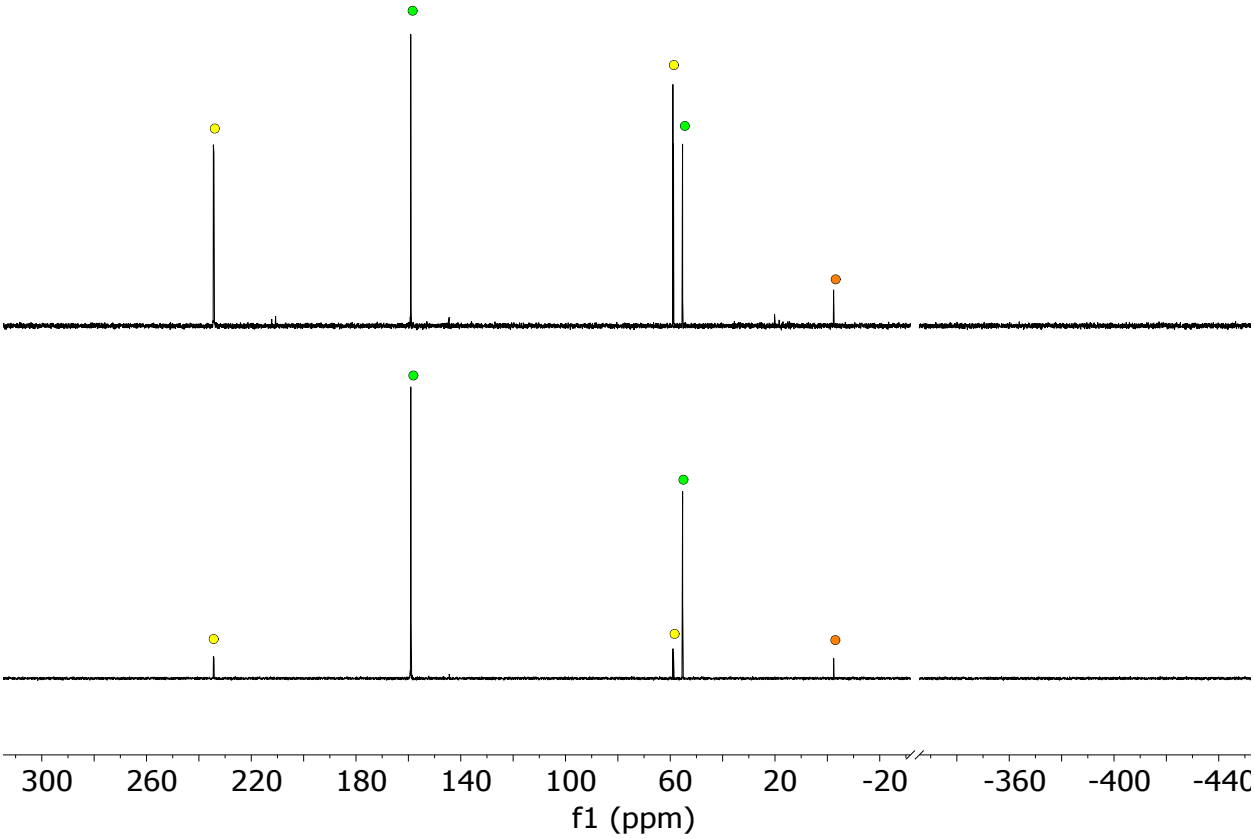
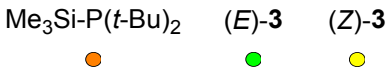
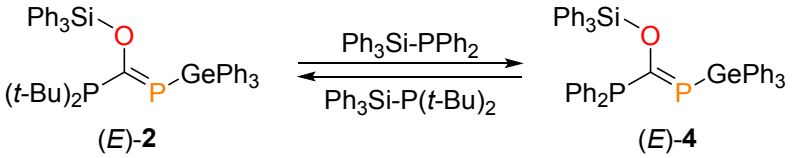


Figure 16. Stacked $^{31}P\{^1H\}$ NMR spectra of *in-situ* formation of (*E*)-**3**/(*Z*)-**3** (THF)

Bottom: 23 °C, 30 min. Top: 70 °C, 1 h.



Reaction of (*E*)-**2** with Ph_2P-$SiPh_3$



(*E*)-**2** (*E*)-**4**

A solution of (*E*)-**2** (18.3 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL) was combined with a solution of Ph_2P-$SiPh_3$ (9.6 mg, 0.02 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL). The homogenous yellow solution was transferred to an NMR tube and analyzed by $^{31}P\{^1H\}$ NMR spectroscopy. Analysis after 30 minutes at ambient temperature showed a mixture of exclusively starting materials. Heating the reaction mixture to 85 °C for 1.5 h showed both phosphine exchange and thermal isomerization, both characterized by the formation of (*Z*)-**2**, (*E*)-**4** and (*Z*)-**4**.

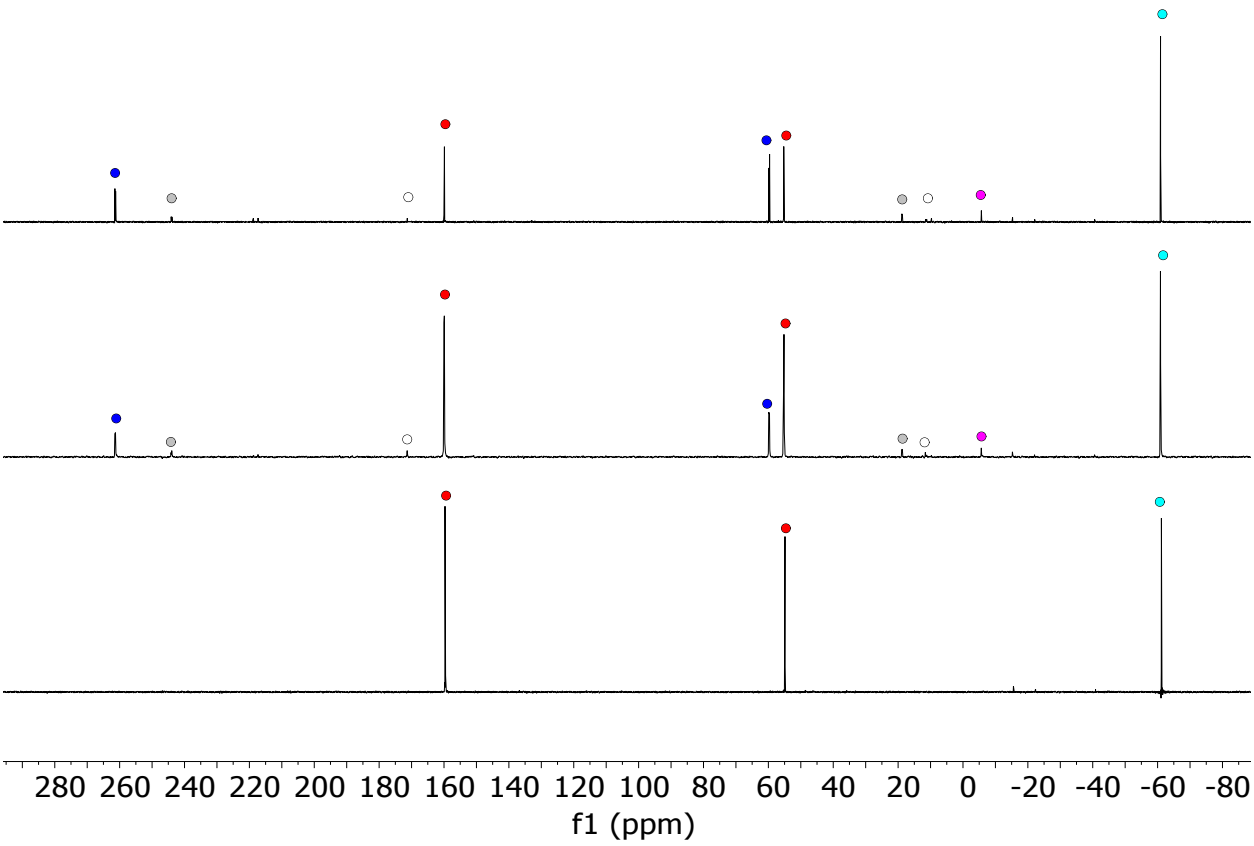
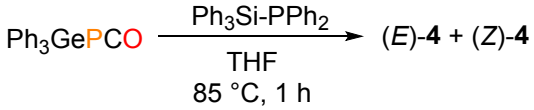


Figure 17. Stacked $^{31}P\{^1H\}$ NMR spectra of displaying phosphine exchange (THF)

Bottom: 23 °C, 30 min. Middle: 85 °C, 1 h. Top: 85 °C, 2 h.

Ph_3Si-$P(t\text{-}Bu)_2$ Ph_3Si-PPh_2 (*E*)-**2** (*Z*)-**2** (*E*)-**4** (*Z*)-**4**

Independent *in-situ* syntheses and characterization of (*E*)-**4**/(*Z*)-**4**



Equimolar solutions of Ph_3GePCO (7.1 mg, 0.02 mmol, 1 equiv.) and $Ph_2P\text{-}SiPh_3$ (8.7 mg, 0.02 mmol, 1 equiv.) were combined in tetrahydrofuran (*ca.* 0.6 mL). The pale-yellow reaction mixture was transferred to an NMR tube and analyzed by $^{31}P\{^1H\}$ NMR spectroscopy, which showed trace amounts of (*E*)-**4** (δ 171 ppm, 11 ppm, $^2J_{PP}$ = 16 Hz). Heating to 85 °C for 1 hour is accompanied by a colour change to bright yellow and increased formation of both (*E*)-**4** and (*Z*)-**4** (δ 244 ppm, 19 ppm, $^2J_{PP}$ = 33 Hz), consistent with thermal isomerization.

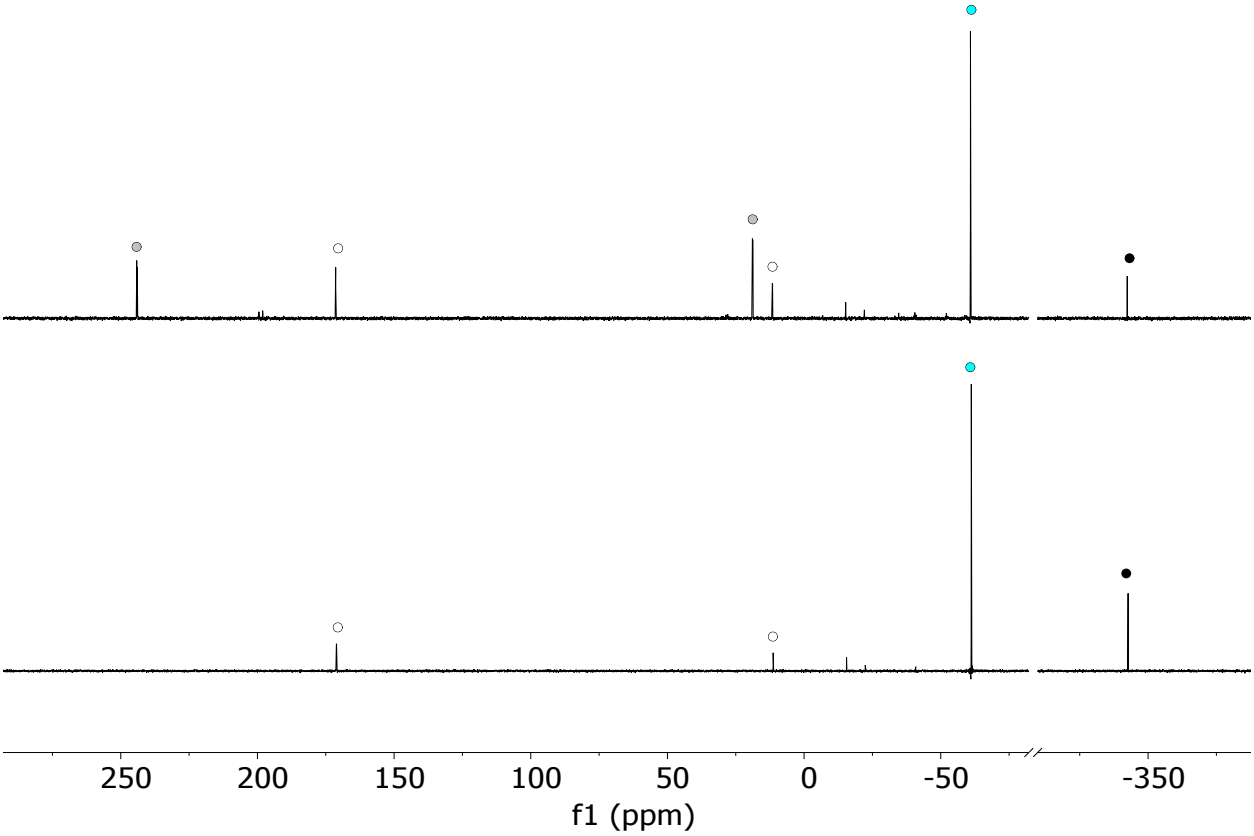
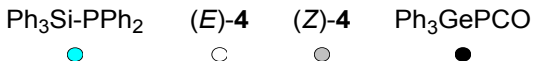
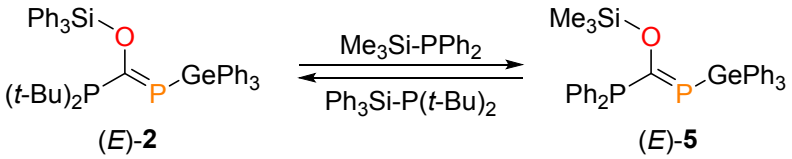


Figure 18. Stacked $^{31}P\{^1H\}$ NMR spectra of *in-situ* formation of (*E*)-**4**/(*Z*)-**4** (THF)

Bottom: 23 °C, 30 min. Top: 85 °C, 1 h.



Reaction of (*E*)-**2** with Ph_2P-$SiMe_3$



A solution of (*E*)-**2** (24.0 mg, 0.031 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL) was combined with a solution of Ph_2P-$SiMe_3$ (8.1 mg, 0.031 mmol, 1 equiv.) in tetrahydrofuran (0.3 mL). The homogenous yellow solution was transferred to an NMR tube and analyzed by $^{31}P\{^1H\}$ NMR spectroscopy. Analysis after 30 minutes at ambient temperature showed the formation of (*Z*)-**2**, small amounts of (*E*)-**5** (δ 225 ppm, 17 ppm, $^2J_{PP}$ = 31 Hz) and (*Z*)-**5** (δ 159 ppm, 11 ppm, $^2J_{PP}$ = 28 Hz) and *t*-Bu_2P-$SiPh_3$.

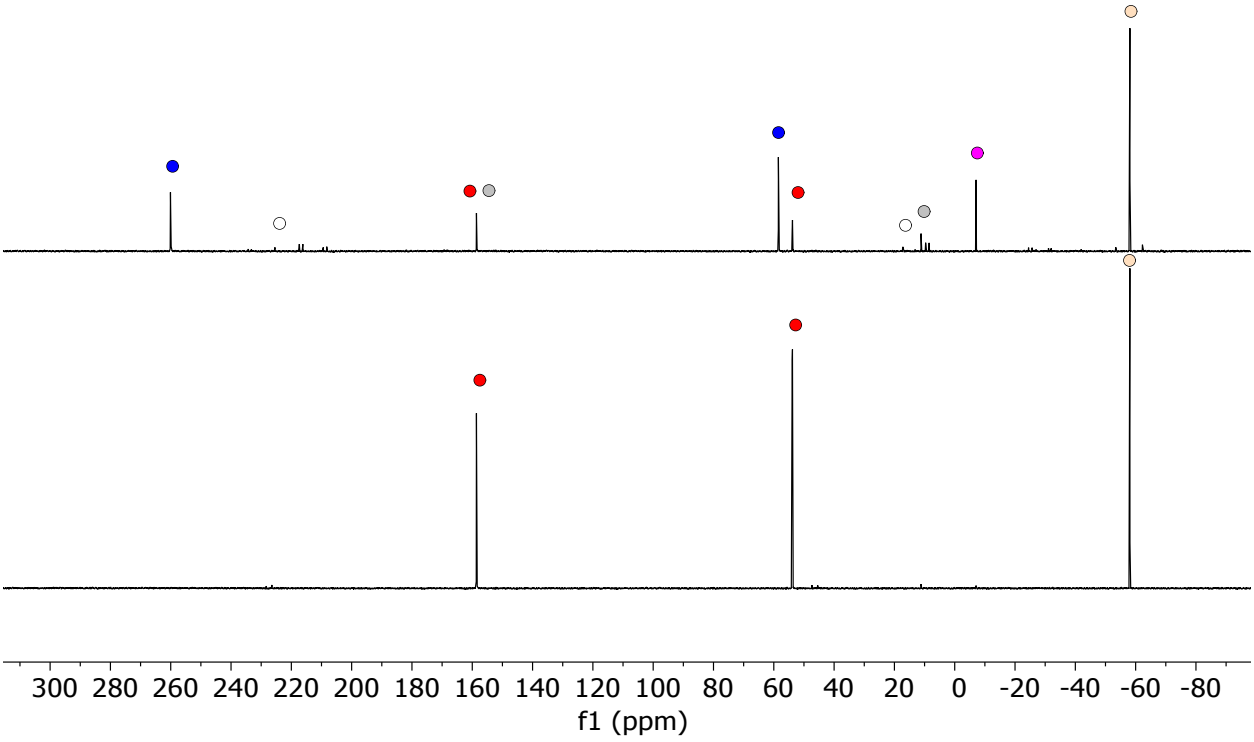
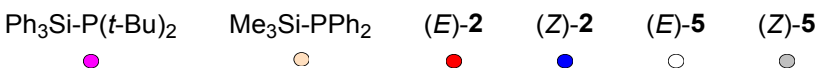
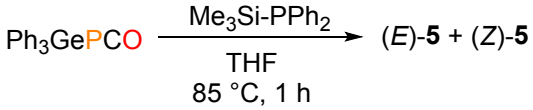


Figure 19. Stacked $^{31}P\{^1H\}$ NMR spectra of displaying silylphosphine exchange (THF)

Bottom: 23 °C, 30 min. Top: 85 °C, 1.5 h.



Independent *in-situ* syntheses and characterization of (*E*)-**5**/(*Z*)-**5**



Equimolar solutions of Ph_3GePCO (17.0 mg, 0.047 mmol, 1 equiv.) and $Ph_2P\text{-}SiMe_3$ (12.1 mg, 0.047 mmol, 1 equiv.) were combined in tetrahydrofuran (*ca.* 0.6 mL). The pale-yellow reaction mixture was transferred to an NMR tube and analyzed by $^{31}P\{^1H\}$ NMR spectroscopy, which showed the formation of (*E*)-**5** and (*Z*)-**5**. Heating to 85 °C for 1 hour is accompanied by the appearance of multiple unidentified products.

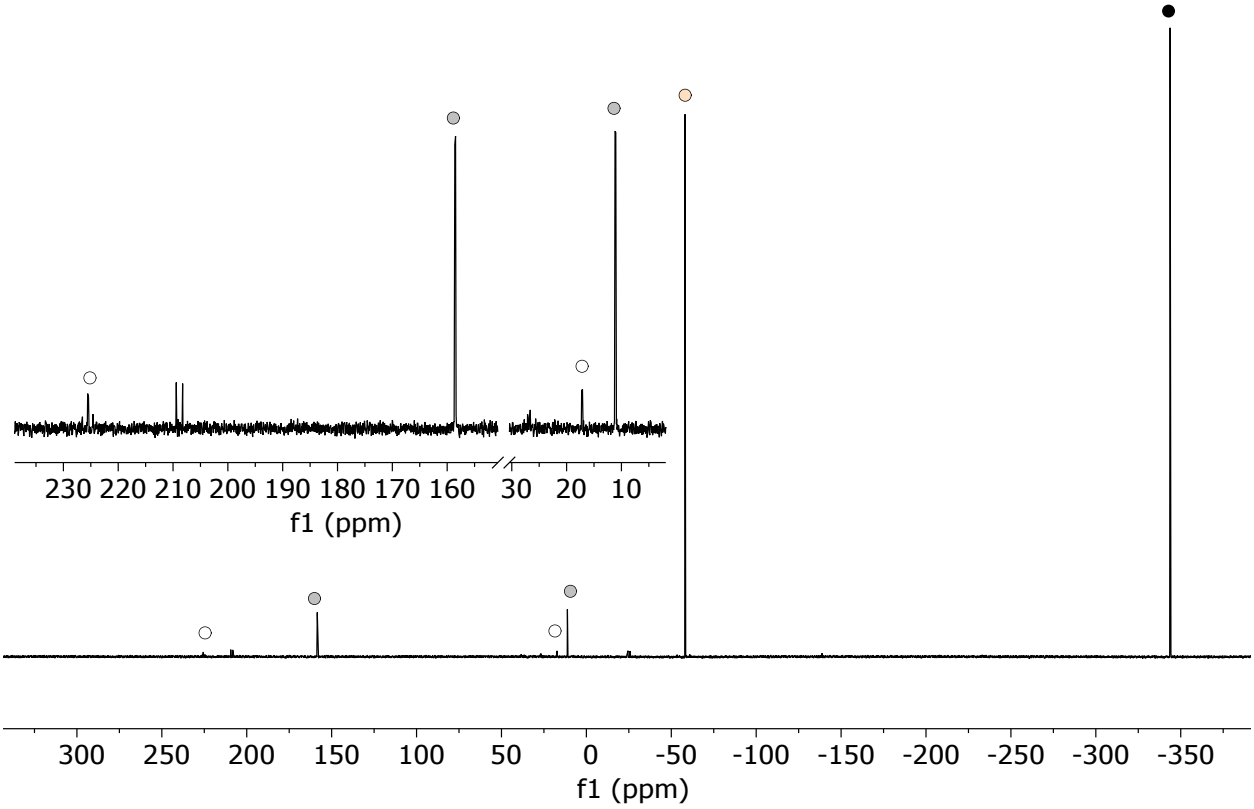
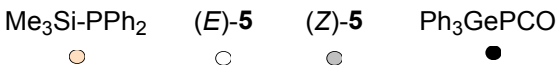


Figure 20. $^{31}P\{^1H\}$ NMR spectrum of *in-situ* formation of (*E*)-**5**/(*Z*)-**5** (THF)



Computational details

Electronic structure calculations, including geometry optimizations and frequency calculations, were performed using Gaussian 09[3] using an ultrafine grid.[4] The structures of (*E*)-**2** and (*Z*)-**2** were optimized at multiple levels of theory (see below), using the coordinates from the crystal structures as a starting point. All structures were confirmed as minima on the potential energy hypersurface by the absence of any imaginary frequencies.

Calculations were initially carried out by carrying out a geometry optimization and frequency analysis using the ωB97X-D functional and the 6-31G* basis set. Single point energy calculations were subsequently carried out at the ωB97X-D/6-311+G** level of theory. These calculations showed that (*E*)-**2** is lower in energy (Table 1).

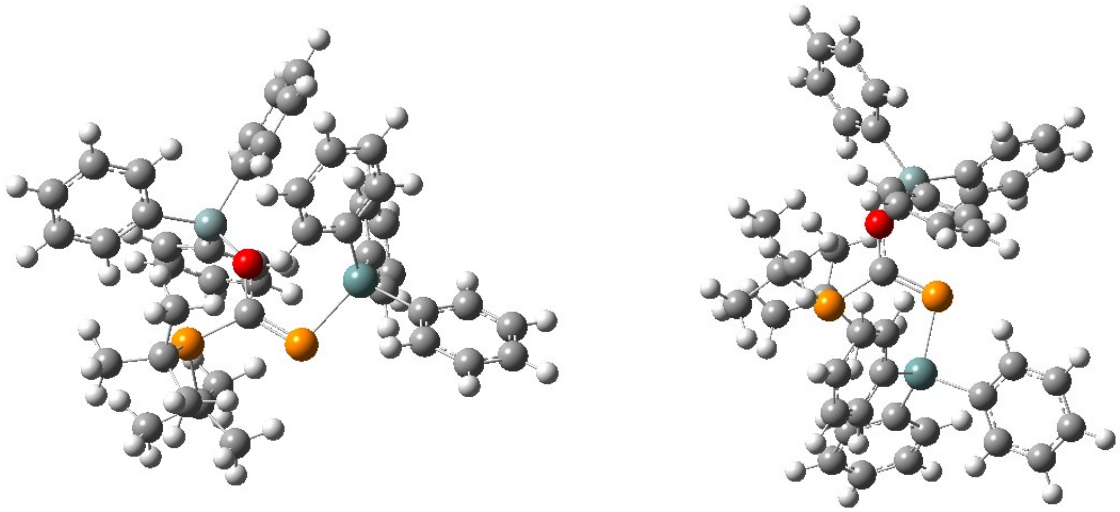


Figure 21. Optimised structures of (*E*)-**2** (left) and (*Z*)-**2** (right) (ωB97X-D/6-31G*).

Table 1. Electronic energies and Gibbs free energy of (*E*)-**2** and (*Z*)-**2**.

	(*E*)-**2**	(*Z*)-**2**
Electronic energy (Hartrees)	-4868.104533	-4868.097513
Electronic energy (kcal/mol)	-3054779.407	-3054775.002
Relative electronic energy (kcal/mol)	**0**	**+4.4**
Thermal correction to Gibbs free energy (Hartrees)	0.734237	0.732010
Thermal correction to Gibbs free energy (kcal/mol)	460.740	459.343
Gibbs free energy (kcal/mol)	-3054318.667	-3054315.659
Relative Gibbs free energy (kcal/mol)	**0**	**+3.0**

The calculations were subsequently carried at alternative and higher levels of theory. In all cases below the geometry optimizations, frequency calculations and single point energies were determined using the following methods:

A) ωB97X-D/6-311+G**

B) ωB97X-D/6-311+G** with solvent correction (THF)

C) M06-2x/6-311+G** with solvent correction (THF) and Grimme's D3 dispersion correction

The results of these are tabulated in Table 2. Again, in all cases, the *Z*-isomer is slightly higher in energy than the *E*-isomer.

Table 2. Electronic energies and Gibbs free energy of (*E*)-**2** and (*Z*)-**2** using methods A, B and C.

	Method A		Method B		Method C	
	(*E*)-**2**	(*Z*)-**2**	(*E*)-**2**	(*Z*)-**2**	(*E*)-**2**	(*Z*)-**2**
Electronic energy (Hartrees)	-4868.105011	-4868.097988	-4868.114859	-4868.109711	-4867.85354	-4867.850797
Electronic energy (kcal/mol)	-3054779.707	-3054775.300	-3054785.887	-3054782.656	-3054621.907	-3054620.186
Relative electronic energy (kcal/mol)	**0**	**+4.4**	**0**	**+3.2**	**0**	**+1.7**
Gibbs free energy (Hartrees)	-4867.379895	-4867.375553	-4867.391276	-4867.386510	-4867.13016	-4867.128092
Gibbs free energy (kcal/mol)	-3054324.691	-3054321.966	-3054331.832	-3054328.842	-3054167.98	-3054166.682
Relative Gibbs free energy (kcal/mol)	**0**	**+2.7**	**0**	**+3.0**	**0**	**+1.30**

Table 3. Cartesian coordinates of optimised structure of (*E*)-**2** (ωB97X-D/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	5.869114	5.386343	4.270061
2	15	0	6.663494	9.865631	2.191998
3	14	0	4.962580	9.785579	5.060221
4	15	0	6.774570	6.728057	2.591051
5	8	0	5.329540	8.444896	4.054555
6	6	0	6.208132	8.267644	3.047894
7	6	0	8.527564	9.827471	1.834835
8	6	0	5.629886	9.783913	0.593778
9	6	0	4.221804	9.302919	0.987443
10	6	0	9.157645	8.664730	1.057403
11	6	0	8.839827	11.138725	1.089564
12	6	0	9.181615	9.890267	3.228088
13	6	0	6.174287	8.877034	-0.513369
14	6	0	5.498678	11.224393	0.065526
15	1	0	3.799359	9.885733	1.812363
16	1	0	4.225728	8.246823	1.271286
17	1	0	3.554020	9.414296	0.123764
18	1	0	10.235494	8.854821	0.962564
19	1	0	9.031199	7.711288	1.573580
20	1	0	8.752754	8.559341	0.049491
21	1	0	8.370588	12.007663	1.565286
22	1	0	9.924891	11.302161	1.088070
23	1	0	8.516123	11.097207	0.044274
24	1	0	8.822495	10.741929	3.815897
25	1	0	10.269019	9.988008	3.113118
26	1	0	8.987269	8.978412	3.801689
27	1	0	6.388857	7.867366	-0.147356
28	1	0	5.427881	8.793816	-1.314805

29	1	0	7.084908	9.287954	-0.959835
30	1	0	5.030667	11.877533	0.808671
31	1	0	4.863773	11.224140	-0.830260
32	1	0	6.462385	11.657950	-0.216033
33	6	0	6.613218	5.856187	6.009484
34	6	0	5.832777	6.218749	7.110044
35	6	0	8.007616	5.843444	6.158576
36	6	0	6.426441	6.568638	8.322030
37	1	0	4.750402	6.248971	7.025512
38	6	0	8.605051	6.185788	7.367731
39	1	0	8.637196	5.561191	5.317221
40	6	0	7.811240	6.555401	8.452633
41	1	0	5.798949	6.862686	9.157651
42	1	0	9.687339	6.167369	7.462711
43	1	0	8.272916	6.833064	9.395916
44	6	0	6.478636	3.573758	3.857014
45	6	0	6.304302	3.058462	2.567256
46	6	0	7.055328	2.746282	4.825240
47	6	0	6.694126	1.760793	2.250840
48	1	0	5.853992	3.678878	1.794702
49	6	0	7.447774	1.445188	4.516725
50	1	0	7.205603	3.120819	5.834856
51	6	0	7.268417	0.950744	3.228194
52	1	0	6.550888	1.381482	1.242963
53	1	0	7.894328	0.818322	5.283667
54	1	0	7.575242	-0.062623	2.984927
55	6	0	3.922432	5.335849	4.274277
56	6	0	3.248336	4.570323	5.231034
57	6	0	3.166025	6.003653	3.308352
58	6	0	1.858120	4.492032	5.237555
59	1	0	3.812791	4.025401	5.984660
60	6	0	1.775495	5.927872	3.304006
61	1	0	3.669036	6.604789	2.556338
62	6	0	1.118309	5.175391	4.274987
63	1	0	1.352478	3.896402	5.992516
64	1	0	1.206141	6.457974	2.545684
65	1	0	0.033612	5.114750	4.276607
66	6	0	6.557284	10.425816	5.787134
67	6	0	6.834292	11.783664	5.993739
68	6	0	7.502791	9.482932	6.217105
69	6	0	8.029850	12.187528	6.583303
70	1	0	6.111601	12.538217	5.695524
71	6	0	8.694132	9.881884	6.812891
72	1	0	7.313039	8.422311	6.079605
73	6	0	8.963369	11.236719	6.989367
74	1	0	8.231026	13.245047	6.728998
75	1	0	9.408863	9.130333	7.134739
76	1	0	9.895836	11.552429	7.448853
77	6	0	3.906037	11.106357	4.237395
78	6	0	4.448837	12.205659	3.552510
79	6	0	2.507872	11.024167	4.327018
80	6	0	3.632899	13.173753	2.976420
81	1	0	5.525316	12.289095	3.443796
82	6	0	1.685759	11.979719	3.733844
83	1	0	2.046503	10.206743	4.873185
84	6	0	2.246950	13.057583	3.057300
85	1	0	4.080195	14.015572	2.455208
86	1	0	0.606446	11.884237	3.808948
87	1	0	1.608558	13.807255	2.598505
88	6	0	3.956258	8.984101	6.419534
89	6	0	4.236528	9.285885	7.758909
90	6	0	2.903390	8.097357	6.151048
91	6	0	3.497584	8.718801	8.794331
92	1	0	5.056099	9.957340	8.001405
93	6	0	2.162781	7.526250	7.181812
94	1	0	2.666658	7.824713	5.127044
95	6	0	2.462379	7.833249	8.507276
96	1	0	3.735564	8.963610	9.825857
97	1	0	1.362727	6.832246	6.944191
98	1	0	1.888953	7.384770	9.313779

Table 4. Cartesian coordinates of optimised structure of (*Z*)-**2** (ωB97X-D/6-31G*).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	2.509873	8.919275	2.698094
2	15	0	1.595891	5.570601	2.750857
3	15	0	1.115233	8.181538	4.422494
4	14	0	0.733367	6.077388	7.002157
5	8	0	0.723222	5.718665	5.335678
6	6	0	2.649166	10.834499	3.097688
7	6	0	2.510573	4.013789	3.335112
8	6	0	0.484740	4.387936	7.759436
9	6	0	1.858696	8.727394	0.871356
10	6	0	-0.696363	7.201034	7.421836
11	6	0	-0.613181	2.218011	7.713142
12	1	0	-1.270434	1.511602	7.214474
13	6	0	1.145595	6.477854	4.298874
14	6	0	2.379689	6.818973	7.493593
15	6	0	4.309384	8.209347	2.957705
16	6	0	2.541406	8.204879	7.648587
17	1	0	1.681560	8.860878	7.544907
18	6	0	-0.147891	5.115987	2.119123
19	6	0	-0.367326	3.461128	7.139966
20	1	0	-0.839453	3.713540	6.193374
21	6	0	0.790376	9.521850	0.441312
22	1	0	0.367175	10.266615	1.111779
23	6	0	3.513340	6.004238	7.630181
24	1	0	3.420824	4.925723	7.525770
25	6	0	2.369915	7.772331	-0.013483
26	1	0	3.173178	7.116563	0.308468
27	6	0	3.625560	4.522481	4.263801
28	1	0	4.265230	5.255840	3.764230
29	1	0	3.224993	4.986947	5.168125
30	1	0	4.256856	3.678042	4.570669
31	6	0	-1.751178	7.415567	6.525753
32	1	0	-1.714112	6.975137	5.532689
33	6	0	4.738683	7.808487	4.227690
34	1	0	4.044603	7.805202	5.064685
35	6	0	3.791096	8.756379	7.914573
36	1	0	3.896894	9.832020	8.020967
37	6	0	0.004927	4.065731	1.007211
38	1	0	0.747733	4.372737	0.261882
39	1	0	0.288535	3.084300	1.398974
40	1	0	-0.955654	3.946738	0.489586
41	6	0	1.838980	7.621975	-1.291663
42	1	0	2.251065	6.874516	-1.963870
43	6	0	-0.016530	1.881103	8.926413
44	1	0	-0.206684	0.910364	9.375212
45	6	0	3.193052	3.412294	2.090881
46	1	0	3.795476	4.162046	1.566067
47	1	0	3.862814	2.600266	2.403340
48	1	0	2.477055	2.991317	1.379518
49	6	0	-0.722055	6.393376	1.482323
50	1	0	-0.123537	6.723968	0.629245
51	1	0	-1.740569	6.190447	1.125641
52	1	0	-0.778125	7.219293	2.199178
53	6	0	-0.769950	7.797218	8.688467
54	1	0	0.034944	7.649223	9.406154
55	6	0	1.710935	2.924487	4.056678
56	1	0	1.214037	3.311961	4.948000
57	1	0	0.959399	2.465172	3.406940
58	1	0	2.394616	2.125052	4.373668
59	6	0	0.247708	9.371096	-0.832535
60	1	0	-0.587044	9.993002	-1.142895
61	6	0	2.980323	13.555380	3.731228
62	1	0	3.105167	14.606519	3.975721

63	6	0	2.781329	11.255671	4.426672
64	1	0	2.764816	10.522357	5.230889
65	6	0	5.239007	8.195385	1.911961
66	1	0	4.945293	8.528166	0.919443
67	6	0	-2.895486	8.791905	8.140594
68	1	0	-3.744668	9.410473	8.416532
69	6	0	0.773687	8.420226	-1.702927
70	1	0	0.352938	8.298901	-2.697060
71	6	0	4.906442	7.929821	8.033764
72	1	0	5.883433	8.360563	8.233120
73	6	0	0.821432	2.791680	9.563288
74	1	0	1.286390	2.534193	10.510568
75	6	0	6.049527	7.392602	4.443857
76	1	0	6.353758	7.082777	5.439434
77	6	0	-1.141367	4.610033	3.174070
78	1	0	-1.358880	5.380765	3.918565
79	1	0	-2.086887	4.347494	2.680443
80	1	0	-0.781824	3.725132	3.703045
81	6	0	1.067491	4.034167	8.983515
82	1	0	1.728776	4.732495	9.491498
83	6	0	-2.841557	8.204057	6.879295
84	1	0	-3.646769	8.364673	6.168443
85	6	0	6.955867	7.363204	3.387640
86	1	0	7.977097	7.031042	3.552187
87	6	0	2.697175	11.806647	2.093621
88	1	0	2.607869	11.511333	1.051184
89	6	0	2.944587	12.600513	4.744625
90	1	0	3.043012	12.904120	5.783241
91	6	0	-1.857990	8.587860	9.046757
92	1	0	-1.895748	9.045609	10.031016
93	6	0	6.548360	7.768272	2.119340
94	1	0	7.251189	7.757494	1.290924
95	6	0	2.859329	13.155436	2.403730
96	1	0	2.892486	13.893376	1.606932
97	6	0	4.765985	6.551374	7.896815
98	1	0	5.630810	5.901564	7.995152

Table 5. Cartesian coordinates of optimised structure of (*E*)-**2** (ωB97X-D/6-311+G**; Method A).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	5.856535	5.387387	4.252425
2	15	0	6.672232	9.868557	2.199846
3	14	0	4.968359	9.785716	5.079295
4	15	0	6.745306	6.734868	2.565679
5	8	0	5.352214	8.449792	4.078814
6	6	0	6.204752	8.270808	3.052106
7	6	0	8.538945	9.818259	1.863056
8	6	0	5.658396	9.796189	0.590135
9	6	0	4.243078	9.331125	0.970551
10	6	0	9.165798	8.648399	1.097536
11	6	0	8.867038	11.123372	1.117539
12	6	0	9.176237	9.879676	3.262001
13	6	0	6.206236	8.884829	-0.509277
14	6	0	5.550529	11.236300	0.059734
15	1	0	3.821015	9.918368	1.790017
16	1	0	4.233779	8.277272	1.254013
17	1	0	3.586380	9.450526	0.102046
18	1	0	10.243610	8.831583	1.010821
19	1	0	9.030514	7.701004	1.618156
20	1	0	8.768911	8.539475	0.089229
21	1	0	8.396478	11.994421	1.583393
22	1	0	9.950953	11.280108	1.130988
23	1	0	8.557460	11.078779	0.070416

24	1	0	8.814447	10.732757	3.842374
25	1	0	10.263232	9.971708	3.158988
26	1	0	8.970575	8.971398	3.833644
27	1	0	6.401301	7.873365	-0.143969
28	1	0	5.470361	8.814227	-1.318971
29	1	0	7.126407	9.284509	-0.940818
30	1	0	5.089357	11.896220	0.797849
31	1	0	4.920112	11.242076	-0.836740
32	1	0	6.519569	11.654351	-0.218052
33	6	0	6.622093	5.863109	5.986975
34	6	0	5.848090	6.190219	7.100346
35	6	0	8.016440	5.874852	6.116738
36	6	0	6.450002	6.525676	8.310077
37	1	0	4.765874	6.204639	7.030179
38	6	0	8.619536	6.205019	7.323765
39	1	0	8.642289	5.624252	5.264634
40	6	0	7.833849	6.534718	8.424086
41	1	0	5.829645	6.790916	9.158519
42	1	0	9.701360	6.207290	7.405160
43	1	0	8.300741	6.800672	9.366189
44	6	0	6.453152	3.564142	3.837778
45	6	0	6.201165	3.025499	2.572307
46	6	0	7.092698	2.761777	4.784705
47	6	0	6.578482	1.725379	2.259916
48	1	0	5.700794	3.625086	1.816402
49	6	0	7.471239	1.458230	4.476662
50	1	0	7.300949	3.153789	5.775511
51	6	0	7.215617	0.938570	3.213916
52	1	0	6.375739	1.325003	1.272462
53	1	0	7.966351	0.848652	5.225034
54	1	0	7.511269	-0.076592	2.972459
55	6	0	3.903346	5.346045	4.261874
56	6	0	3.225769	4.562754	5.198815
57	6	0	3.157028	6.042473	3.311213
58	6	0	1.837208	4.494970	5.198996
59	1	0	3.782776	3.996015	5.939549
60	6	0	1.768231	5.972955	3.302023
61	1	0	3.664347	6.660090	2.577757
62	6	0	1.105556	5.203185	4.251832
63	1	0	1.325814	3.886605	5.937362
64	1	0	1.204111	6.523536	2.556838
65	1	0	0.022257	5.149567	4.249574
66	6	0	6.555370	10.455820	5.798616
67	6	0	6.825965	11.816939	5.970836
68	6	0	7.498201	9.529264	6.259698
69	6	0	8.013769	12.238766	6.558253
70	1	0	6.104903	12.560680	5.649158
71	6	0	8.681900	9.946268	6.852473
72	1	0	7.310733	8.466019	6.152587
73	6	0	8.945346	11.303678	6.995689
74	1	0	8.210381	13.298597	6.678151
75	1	0	9.395842	9.207081	7.198505
76	1	0	9.871871	11.633689	7.452965
77	6	0	3.889386	11.076901	4.239124
78	6	0	4.413132	12.169884	3.535597
79	6	0	2.495467	10.970342	4.328170
80	6	0	3.582344	13.110442	2.941841
81	1	0	5.486224	12.266096	3.421976
82	6	0	1.658871	11.898051	3.716705
83	1	0	2.047609	10.156124	4.886850
84	6	0	2.200976	12.971579	3.022781
85	1	0	4.013941	13.948452	2.405009
86	1	0	0.582995	11.784627	3.791313
87	1	0	1.551130	13.699854	2.549911
88	6	0	3.978915	8.982716	6.451302
89	6	0	4.257213	9.302143	7.784432
90	6	0	2.936539	8.084521	6.194530
91	6	0	3.527399	8.738614	8.825065
92	1	0	5.067655	9.985061	8.018773
93	6	0	2.204372	7.518546	7.230385
94	1	0	2.701894	7.798791	5.175687

95	6	0	2.501789	7.842331	8.549859
96	1	0	3.764599	8.995834	9.851868
97	1	0	1.411473	6.815691	7.002015
98	1	0	1.934944	7.397497	9.360688

Table 6. Cartesian coordinates of optimised structure of (*Z*)-**2** (ωB97X-D/6-311+G**; Method A).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	2.517651	8.930367	2.700652
2	15	0	1.594793	5.585849	2.759065
3	15	0	1.142659	8.186174	4.443384
4	14	0	0.737791	6.064188	7.019586
5	8	0	0.743475	5.727156	5.350906
6	6	0	2.647002	10.859320	3.069098
7	6	0	2.523289	4.032311	3.327823
8	6	0	0.482810	4.368332	7.758868
9	6	0	1.854466	8.730632	0.872593
10	6	0	-0.698418	7.180209	7.438225
11	6	0	-0.631474	2.213006	7.691761
12	1	0	-1.295395	1.518797	7.188492
13	6	0	1.162906	6.485921	4.314615
14	6	0	2.382020	6.800436	7.522273
15	6	0	4.323615	8.218546	2.960000
16	6	0	2.541744	8.179403	7.708179
17	1	0	1.682338	8.835711	7.620418
18	6	0	-0.154886	5.125273	2.150924
19	6	0	-0.376480	3.457621	7.131873
20	1	0	-0.846542	3.722973	6.189779
21	6	0	0.804224	9.545211	0.442514
22	1	0	0.400439	10.304960	1.105537
23	6	0	3.514364	5.984447	7.632397
24	1	0	3.422946	4.910610	7.500102
25	6	0	2.346652	7.762478	-0.005375
26	1	0	3.134326	7.091440	0.317369
27	6	0	3.656447	4.548311	4.227727
28	1	0	4.278362	5.281935	3.710236
29	1	0	3.279264	5.012280	5.139795
30	1	0	4.298076	3.708604	4.518393
31	6	0	-1.731018	7.419537	6.527122
32	1	0	-1.674108	7.006615	5.525101
33	6	0	4.760049	7.856705	4.237379
34	1	0	4.075450	7.882259	5.080173
35	6	0	3.789977	8.724290	7.982276
36	1	0	3.896262	9.795450	8.112689
37	6	0	-0.010679	4.080066	1.035209
38	1	0	0.723756	4.389081	0.285412
39	1	0	0.276408	3.099993	1.421737
40	1	0	-0.974607	3.963648	0.527587
41	6	0	1.809637	7.616621	-1.279062
42	1	0	2.204340	6.858938	-1.947516
43	6	0	-0.035330	1.858085	8.897451
44	1	0	-0.232719	0.885951	9.335761
45	6	0	3.179016	3.425031	2.074029
46	1	0	3.765399	4.172059	1.531601
47	1	0	3.858291	2.620675	2.378790
48	1	0	2.450907	2.995877	1.383812
49	6	0	-0.742457	6.401929	1.528608
50	1	0	-0.151667	6.746042	0.677872
51	1	0	-1.758260	6.191449	1.174922
52	1	0	-0.804141	7.218946	2.251983
53	6	0	-0.798620	7.739967	8.716803
54	1	0	-0.012854	7.569972	9.448148
55	6	0	1.737637	2.948835	4.069791
56	1	0	1.252050	3.342570	4.961761
57	1	0	0.980504	2.483240	3.434825

58	1	0	2.427379	2.155998	4.383585
59	6	0	0.255220	9.394504	-0.826361
60	1	0	-0.566892	10.029292	-1.138434
61	6	0	2.995016	13.589809	3.619980
62	1	0	3.127177	14.645095	3.832531
63	6	0	2.657141	11.331267	4.385154
64	1	0	2.530507	10.639036	5.212898
65	6	0	5.238706	8.163544	1.905716
66	1	0	4.939644	8.464855	0.906686
67	6	0	-2.907391	8.751116	8.150482
68	1	0	-3.760522	9.362030	8.424391
69	6	0	0.759193	8.429903	-1.690779
70	1	0	0.333248	8.310060	-2.680931
71	6	0	4.904167	7.897577	8.076837
72	1	0	5.879941	8.324131	8.282189
73	6	0	0.811563	2.752459	9.540068
74	1	0	1.276437	2.480594	10.481361
75	6	0	6.067785	7.438437	4.451970
76	1	0	6.380588	7.158562	5.451932
77	6	0	-1.130398	4.609388	3.215334
78	1	0	-1.339994	5.371937	3.967054
79	1	0	-2.079348	4.348272	2.731810
80	1	0	-0.761064	3.723027	3.730242
81	6	0	1.066306	3.997338	8.974402
82	1	0	1.733915	4.683138	9.487567
83	6	0	-2.826772	8.198189	6.877687
84	1	0	-3.615334	8.378256	6.155525
85	6	0	6.961507	7.367534	3.389946
86	1	0	7.980096	7.033359	3.554754
87	6	0	2.822226	11.783187	2.035526
88	1	0	2.824506	11.447744	1.002901
89	6	0	2.827651	12.683221	4.660429
90	1	0	2.829022	13.029682	5.688433
91	6	0	-1.891488	8.521322	9.071503
92	1	0	-1.950856	8.951035	10.065376
93	6	0	6.544707	7.732883	2.115194
94	1	0	7.238434	7.688962	1.282440
95	6	0	2.993887	13.136749	2.306163
96	1	0	3.127842	13.837913	1.489366
97	6	0	4.765156	6.525380	7.905493
98	1	0	5.630113	5.875584	7.981304

Table 7. Cartesian coordinates of optimised structure of (*E*)-**2** (ωB97X-D/6-311+G**, THF; Method B).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	5.854285	5.384577	4.259484
2	15	0	6.677482	9.870642	2.205660
3	14	0	4.970644	9.788171	5.084340
4	15	0	6.743866	6.731972	2.574062
5	8	0	5.359645	8.448936	4.086129
6	6	0	6.208529	8.271898	3.057962
7	6	0	8.542584	9.816931	1.861526
8	6	0	5.657393	9.805229	0.599862
9	6	0	4.242055	9.342298	0.982529
10	6	0	9.165606	8.643003	1.098994
11	6	0	8.868460	11.117956	1.107575
12	6	0	9.187433	9.883358	3.256702
13	6	0	6.200033	8.896818	-0.504514
14	6	0	5.552503	11.247466	0.074219
15	1	0	3.823316	9.931469	1.802272
16	1	0	4.229949	8.288883	1.268030
17	1	0	3.585196	9.461494	0.114352
18	1	0	10.241010	8.831553	0.997128
19	1	0	9.042069	7.701248	1.633002
20	1	0	8.755883	8.522380	0.097139

21	1	0	8.399566	11.992127	1.569282
22	1	0	9.952474	11.273492	1.117647
23	1	0	8.555810	11.067271	0.061839
24	1	0	8.827418	10.738240	3.835704
25	1	0	10.273669	9.975535	3.146837
26	1	0	8.984110	8.977523	3.833346
27	1	0	6.387453	7.881945	-0.144361
28	1	0	5.463283	8.836248	-1.314003
29	1	0	7.123049	9.292546	-0.933253
30	1	0	5.105796	11.909209	0.819682
31	1	0	4.911013	11.257977	-0.814140
32	1	0	6.520756	11.659188	-0.214970
33	6	0	6.620224	5.855023	5.995245
34	6	0	5.843870	6.180603	7.107872
35	6	0	8.014711	5.872479	6.126265
36	6	0	6.443280	6.518252	8.318751
37	1	0	4.761737	6.192347	7.036004
38	6	0	8.615884	6.206924	7.333613
39	1	0	8.643714	5.626204	5.275223
40	6	0	7.827698	6.533437	8.433739
41	1	0	5.821983	6.782567	9.167031
42	1	0	9.697431	6.218305	7.414871
43	1	0	8.293128	6.803232	9.375410
44	6	0	6.450942	3.561787	3.831566
45	6	0	6.191091	3.029014	2.564185
46	6	0	7.099596	2.754353	4.768958
47	6	0	6.569073	1.730541	2.240951
48	1	0	5.683779	3.630835	1.814561
49	6	0	7.479079	1.452603	4.450861
50	1	0	7.314298	3.140158	5.760814
51	6	0	7.215224	0.939001	3.186209
52	1	0	6.359785	1.335555	1.252673
53	1	0	7.980820	0.839883	5.192201
54	1	0	7.511126	-0.074156	2.936915
55	6	0	3.901143	5.344605	4.266872
56	6	0	3.218559	4.582599	5.218564
57	6	0	3.158683	6.029532	3.304155
58	6	0	1.828961	4.524770	5.220999
59	1	0	3.770322	4.028560	5.972760
60	6	0	1.768880	5.970551	3.297678
61	1	0	3.668851	6.629617	2.558155
62	6	0	1.101388	5.222322	4.262086
63	1	0	1.313628	3.937121	5.973061
64	1	0	1.207814	6.513590	2.544794
65	1	0	0.017727	5.179778	4.264321
66	6	0	6.558706	10.457084	5.803879
67	6	0	6.826555	11.817366	5.989330
68	6	0	7.506223	9.528644	6.252521
69	6	0	8.015658	12.236730	6.577401
70	1	0	6.103824	12.563953	5.678491
71	6	0	8.691282	9.942369	6.846039
72	1	0	7.320909	8.465736	6.135873
73	6	0	8.951753	11.299610	7.002569
74	1	0	8.209584	13.295833	6.707176
75	1	0	9.409702	9.202733	7.182202
76	1	0	9.878766	11.627370	7.460321
77	6	0	3.889278	11.068552	4.232617
78	6	0	4.408724	12.179574	3.554542
79	6	0	2.495572	10.928102	4.276479
80	6	0	3.574626	13.106802	2.943366
81	1	0	5.481537	12.305171	3.474019
82	6	0	1.655969	11.841787	3.647328
83	1	0	2.048480	10.096065	4.808977
84	6	0	2.194500	12.935102	2.980072
85	1	0	4.003002	13.958780	2.426695
86	1	0	0.581397	11.701551	3.685640
87	1	0	1.542788	13.652192	2.493087
88	6	0	3.981007	8.986610	6.458328
89	6	0	4.258665	9.314233	7.790283
90	6	0	2.940382	8.083888	6.208000
91	6	0	3.531912	8.754737	8.835784

92	1	0	5.066640	10.001230	8.021401
93	6	0	2.209186	7.523724	7.248393
94	1	0	2.706192	7.789895	5.191245
95	6	0	2.506817	7.855276	8.566426
96	1	0	3.772056	9.015585	9.860821
97	1	0	1.416506	6.818456	7.026473
98	1	0	1.942119	7.413100	9.380083

Table 8. Cartesian coordinates of optimised structure of (*Z*)-**2** (ωB97X-D/6-311+G**, THF; Method B).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	2.505768	8.925122	2.695827
2	15	0	1.604306	5.549092	2.762130
3	15	0	1.122153	8.164501	4.420425
4	14	0	0.748485	6.071650	7.020162
5	8	0	0.747899	5.712604	5.351746
6	6	0	2.629413	10.848148	3.106888
7	6	0	2.507373	3.987210	3.348857
8	6	0	0.470246	4.385748	7.773591
9	6	0	1.853328	8.740745	0.864133
10	6	0	-0.682124	7.203827	7.418931
11	6	0	-0.669344	2.241884	7.721528
12	1	0	-1.337822	1.549987	7.221182
13	6	0	1.159486	6.461145	4.309137
14	6	0	2.402235	6.798670	7.501742
15	6	0	4.323548	8.237784	2.947311
16	6	0	2.583844	8.179824	7.652306
17	1	0	1.735884	8.849053	7.554730
18	6	0	-0.142395	5.103259	2.133811
19	6	0	-0.395750	3.478110	7.149845
20	1	0	-0.856926	3.737676	6.201688
21	6	0	0.769232	9.517340	0.446419
22	1	0	0.327129	10.243383	1.122598
23	6	0	3.524048	5.969201	7.626974
24	1	0	3.419137	4.893589	7.523405
25	6	0	2.388164	7.809730	-0.029023
26	1	0	3.207492	7.170570	0.280191
27	6	0	3.637454	4.491122	4.259261
28	1	0	4.271950	5.217386	3.746350
29	1	0	3.256506	4.959490	5.167253
30	1	0	4.266111	3.644354	4.556942
31	6	0	-1.753148	7.357333	6.532332
32	1	0	-1.728117	6.867550	5.564126
33	6	0	4.752575	7.801140	4.203881
34	1	0	4.054296	7.745050	5.033906
35	6	0	3.841484	8.713570	7.906734
36	1	0	3.962715	9.785983	8.011109
37	6	0	0.001114	4.040159	1.034807
38	1	0	0.749612	4.325961	0.289637
39	1	0	0.267433	3.061301	1.438086
40	1	0	-0.958614	3.932071	0.517750
41	6	0	1.859063	7.662148	-1.306605
42	1	0	2.285564	6.932500	-1.986439
43	6	0	-0.084656	1.892924	8.935525
44	1	0	-0.295813	0.927765	9.382626
45	6	0	3.167489	3.362520	2.105793
46	1	0	3.767423	4.097580	1.561548
47	1	0	3.834221	2.553296	2.424692
48	1	0	2.440698	2.935903	1.412960
49	6	0	-0.704736	6.377965	1.485890
50	1	0	-0.092997	6.704479	0.642718
51	1	0	-1.716152	6.173155	1.116986
52	1	0	-0.769645	7.204521	2.198131
53	6	0	-0.745623	7.856553	8.655564
54	1	0	0.068338	7.754390	9.367940

55	6	0	1.699431	2.918472	4.088839
56	1	0	1.210067	3.325401	4.972829
57	1	0	0.942568	2.459120	3.449539
58	1	0	2.377079	2.119625	4.413463
59	6	0	0.230591	9.367452	-0.827371
60	1	0	-0.616617	9.972727	-1.130806
61	6	0	2.964805	13.565076	3.738082
62	1	0	3.092102	14.614263	3.981381
63	6	0	2.743348	11.269652	4.436533
64	1	0	2.707076	10.543528	5.244378
65	6	0	5.256602	8.287486	1.907191
66	1	0	4.962343	8.644928	0.925151
67	6	0	-2.892935	8.791585	8.094631
68	1	0	-3.745966	9.408840	8.354046
69	6	0	0.776472	8.438984	-1.707262
70	1	0	0.357809	8.318611	-2.700426
71	6	0	4.944590	7.873062	8.015564
72	1	0	5.927744	8.289654	8.204863
73	6	0	0.768955	2.784862	9.574642
74	1	0	1.224838	2.517672	10.521563
75	6	0	6.071713	7.413243	4.412361
76	1	0	6.379980	7.074253	5.395420
77	6	0	-1.136579	4.616510	3.194356
78	1	0	-1.343191	5.393380	3.932114
79	1	0	-2.083425	4.362661	2.703437
80	1	0	-0.786376	3.732302	3.725853
81	6	0	1.041646	4.021416	8.997589
82	1	0	1.712601	4.704829	9.509270
83	6	0	-2.849547	8.144234	6.863965
84	1	0	-3.667900	8.255931	6.161381
85	6	0	6.984432	7.449427	3.363998
86	1	0	8.011647	7.140208	3.523668
87	6	0	2.695411	11.815790	2.100645
88	1	0	2.618679	11.521701	1.058475
89	6	0	2.908085	12.614120	4.752131
90	1	0	2.992524	12.919563	5.789560
91	6	0	-1.839646	8.646600	8.991486
92	1	0	-1.869850	9.149450	9.951733
93	6	0	6.574441	7.888804	2.109443
94	1	0	7.281788	7.926496	1.287959
95	6	0	2.860386	13.162981	2.411122
96	1	0	2.908422	13.898402	1.615143
97	6	0	4.784593	6.498643	7.879223
98	1	0	5.640614	5.838739	7.966002

Table 9. Cartesian coordinates of optimised structure of (*E*)-**2** (M06-2x/6-311+G**, THF, GD3; Method C).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	5.825412	5.400003	4.236093
2	15	0	6.688527	9.875496	2.235535
3	14	0	4.939987	9.736998	5.087909
4	15	0	6.738742	6.727036	2.533882
5	8	0	5.345299	8.407275	4.088245
6	6	0	6.203440	8.256748	3.054466
7	6	0	8.559976	9.801783	1.925563
8	6	0	5.717105	9.821376	0.598151
9	6	0	4.295558	9.345376	0.933554
10	6	0	9.199891	8.604761	1.212893
11	6	0	8.902753	11.079490	1.140662
12	6	0	9.182637	9.904193	3.327147
13	6	0	6.295545	8.932293	-0.502287
14	6	0	5.618104	11.269756	0.090684
15	1	0	3.856687	9.912326	1.759398

16	1	0	4.284287	8.284780	1.188731
17	1	0	3.661610	9.487768	0.052428
18	1	0	10.255430	8.842921	1.037744
19	1	0	9.162748	7.705692	1.825771
20	1	0	8.744913	8.381586	0.249527
21	1	0	8.418788	11.965008	1.562905
22	1	0	9.985327	11.235817	1.179372
23	1	0	8.620299	10.994053	0.089128
24	1	0	8.819499	10.777838	3.876314
25	1	0	10.270748	9.982103	3.228809
26	1	0	8.959286	9.014178	3.921222
27	1	0	6.461029	7.909666	-0.154438
28	1	0	5.585626	8.894541	-1.336241
29	1	0	7.235277	9.330501	-0.889436
30	1	0	5.142182	11.913776	0.833356
31	1	0	5.004185	11.285735	-0.816160
32	1	0	6.591489	11.692473	-0.160134
33	6	0	6.637423	5.879130	5.958031
34	6	0	5.901999	6.215019	7.097474
35	6	0	8.038126	5.897014	6.036269
36	6	0	6.549404	6.566255	8.282840
37	1	0	4.816575	6.222876	7.067544
38	6	0	8.686203	6.246626	7.216217
39	1	0	8.632790	5.640298	5.163227
40	6	0	7.938600	6.585688	8.343135
41	1	0	5.962267	6.834913	9.153527
42	1	0	9.769644	6.259079	7.256392
43	1	0	8.439079	6.865926	9.263015
44	6	0	6.402617	3.560422	3.817665
45	6	0	6.157674	3.033957	2.543288
46	6	0	7.029431	2.744064	4.764091
47	6	0	6.526796	1.731131	2.222144
48	1	0	5.670758	3.646118	1.788178
49	6	0	7.400263	1.437722	4.448165
50	1	0	7.233381	3.127276	5.759372
51	6	0	7.149923	0.930316	3.176947
52	1	0	6.330215	1.340532	1.230200
53	1	0	7.884247	0.817739	5.194319
54	1	0	7.439046	-0.084608	2.929671
55	6	0	3.864260	5.411637	4.250042
56	6	0	3.158616	4.678526	5.209775
57	6	0	3.142536	6.115955	3.282700
58	6	0	1.765914	4.668814	5.215790
59	1	0	3.694571	4.110830	5.965905
60	6	0	1.750086	6.103927	3.278956
61	1	0	3.673722	6.694253	2.534068
62	6	0	1.059863	5.385625	4.252718
63	1	0	1.232084	4.104859	5.972519
64	1	0	1.205326	6.659415	2.523779
65	1	0	-0.024077	5.379819	4.257875
66	6	0	6.520143	10.444727	5.787975
67	6	0	6.772966	11.812011	5.951303
68	6	0	7.474626	9.530745	6.255871
69	6	0	7.958570	12.253093	6.534265
70	1	0	6.041012	12.544894	5.629782
71	6	0	8.656275	9.967208	6.845562
72	1	0	7.295664	8.463242	6.157843
73	6	0	8.903573	11.331076	6.977530
74	1	0	8.142229	13.315352	6.647065
75	1	0	9.381372	9.241416	7.196873
76	1	0	9.825928	11.675417	7.431082
77	6	0	3.832206	10.988110	4.226394
78	6	0	4.326691	12.104900	3.536168
79	6	0	2.441494	10.809410	4.265576
80	6	0	3.469072	13.001571	2.907691
81	1	0	5.396663	12.259535	3.461837
82	6	0	1.579790	11.691436	3.617907
83	1	0	2.015071	9.973319	4.808353
84	6	0	2.092720	12.790995	2.938319
85	1	0	3.875708	13.858973	2.383244
86	1	0	0.509822	11.522476	3.651976

87	1	0	1.424789	13.482776	2.438240
88	6	0	3.984670	8.939274	6.490573
89	6	0	4.313428	9.266867	7.813027
90	6	0	2.932843	8.035914	6.279700
91	6	0	3.624995	8.709138	8.887092
92	1	0	5.130682	9.952483	8.013043
93	6	0	2.238250	7.480105	7.349981
94	1	0	2.659517	7.740338	5.272186
95	6	0	2.586682	7.812140	8.657061
96	1	0	3.904152	8.970317	9.901627
97	1	0	1.433149	6.779919	7.160476
98	1	0	2.050576	7.373741	9.491037

Table 10. Cartesian coordinates of optimised structure of (*Z*)-**2** (M06-2x/6-311+G**, THF, GD3; Method C).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	32	0	2.498290	8.917254	2.704566
2	15	0	1.599112	5.580376	2.741196
3	15	0	1.106787	8.172297	4.445717
4	14	0	0.762817	6.053167	7.005287
5	8	0	0.733036	5.695998	5.338713
6	6	0	2.596681	10.853112	3.098209
7	6	0	2.480660	4.005671	3.324463
8	6	0	0.501956	4.371278	7.771671
9	6	0	1.872635	8.712308	0.857114
10	6	0	-0.656422	7.190843	7.427005
11	6	0	-0.649443	2.231685	7.741322
12	1	0	-1.330008	1.542208	7.255397
13	6	0	1.144528	6.468656	4.305384
14	6	0	2.414685	6.791730	7.480315
15	6	0	4.315674	8.216630	2.986743
16	6	0	2.578186	8.175284	7.642998
17	1	0	1.720504	8.832794	7.543039
18	6	0	-0.149216	5.148882	2.111994
19	6	0	-0.380042	3.467149	7.162809
20	1	0	-0.856594	3.731988	6.222911
21	6	0	0.806470	9.499301	0.409274
22	1	0	0.366382	10.243076	1.068006
23	6	0	3.544264	5.971731	7.611282
24	1	0	3.449302	4.895255	7.502245
25	6	0	2.408873	7.757847	-0.013267
26	1	0	3.211978	7.110403	0.322512
27	6	0	3.610563	4.504878	4.236773
28	1	0	4.266443	5.201751	3.709559
29	1	0	3.226545	5.008930	5.125427
30	1	0	4.212843	3.650188	4.563463
31	6	0	-1.709186	7.407091	6.530703
32	1	0	-1.672755	6.964411	5.540103
33	6	0	4.737496	7.791818	4.252424
34	1	0	4.036126	7.752769	5.083068
35	6	0	3.829007	8.722036	7.912682
36	1	0	3.937909	9.794274	8.027817
37	6	0	-0.012732	4.074460	1.024821
38	1	0	0.744263	4.346933	0.283144
39	1	0	0.238404	3.096987	1.439096
40	1	0	-0.971198	3.977567	0.504243
41	6	0	1.898223	7.597960	-1.298382
42	1	0	2.324993	6.853168	-1.960564
43	6	0	-0.043354	1.882206	8.946251
44	1	0	-0.250758	0.919163	9.398157
45	6	0	3.142041	3.377517	2.084921
46	1	0	3.739626	4.113572	1.539926
47	1	0	3.810591	2.573554	2.411040

48	1	0	2.416424	2.945863	1.394896
49	6	0	-0.697176	6.421640	1.450110
50	1	0	-0.087552	6.723549	0.595663
51	1	0	-1.714962	6.223970	1.096412
52	1	0	-0.740844	7.258912	2.151717
53	6	0	-0.725809	7.785351	8.693473
54	1	0	0.076363	7.632013	9.410636
55	6	0	1.665665	2.941374	4.062141
56	1	0	1.187756	3.348574	4.952534
57	1	0	0.901655	2.492333	3.424915
58	1	0	2.341425	2.136937	4.375415
59	6	0	0.283577	9.334925	-0.871332
60	1	0	-0.549919	9.946008	-1.198096
61	6	0	2.880343	13.581025	3.714402
62	1	0	2.986921	14.633239	3.951582
63	6	0	2.664414	11.287964	4.428048
64	1	0	2.611177	10.567100	5.240263
65	6	0	5.252307	8.241014	1.946438
66	1	0	4.962493	8.589904	0.959767
67	6	0	-2.847927	8.787155	8.144954
68	1	0	-3.693211	9.406914	8.420717
69	6	0	0.831030	8.383828	-1.727803
70	1	0	0.426455	8.253153	-2.724833
71	6	0	4.941398	7.891429	8.024585
72	1	0	5.917732	8.317158	8.226417
73	6	0	0.826011	2.771481	9.570358
74	1	0	1.296468	2.502808	10.508975
75	6	0	6.054129	7.391713	4.467516
76	1	0	6.358987	7.063601	5.454967
77	6	0	-1.144156	4.687746	3.180945
78	1	0	-1.356670	5.489734	3.889860
79	1	0	-2.085707	4.413337	2.691877
80	1	0	-0.788316	3.825347	3.743493
81	6	0	1.094602	4.007417	8.986637
82	1	0	1.776096	4.690493	9.484658
83	6	0	-2.797544	8.198586	6.884027
84	1	0	-3.602473	8.359833	6.176470
85	6	0	6.968703	7.401237	3.418179
86	1	0	7.991032	7.081375	3.583677
87	6	0	2.682882	11.813005	2.083983
88	1	0	2.642862	11.507558	1.042939
89	6	0	2.804137	12.638356	4.736505
90	1	0	2.853139	12.954591	5.772343
91	6	0	-1.810933	8.580280	9.050898
92	1	0	-1.847431	9.037758	10.032676
93	6	0	6.566221	7.828070	2.155594
94	1	0	7.274775	7.845025	1.335324
95	6	0	2.822410	13.166085	2.387252
96	1	0	2.886555	13.895035	1.587349
97	6	0	4.798349	6.514550	7.877885
98	1	0	5.660658	5.864193	7.970211

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