Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

A Square Planar Silylene Nickel Four-Membered Ring

Sebastian Kaufmann, Ralf Köppe and Peter W. Roesky

Content

Experimental

General Procedures

All manipulations were performed under exclusion of moisture and oxygen in flame-dried Schlenk-type glassware or in an argon-filled *MBraun* glovebox. THF was distilled under nitrogen from potassium/benzophenone prior to use. The IR spectra were recorded with a Bruker FTIR spectrometer Tensor 37 using a DTGS detector with as CsI window. For the mid (4000 to 400 cm^{-1}) and far (1500 to 200 cm^{-1}) infrared ranges beamsplitters made of KBr and silicon were used. Samples were measured by using the attenuated total reflection (ATR, diamond) technique on bulk material. The Raman spectra were recorded with a Bruker Raman microscope Senterra II using an excitation laser with wavelengths of 532 or 785 nm. Elemental analyses were carried out with a Micro Cube from Elementar Analysensysteme GmbH. Because of the air-sensitive nature of some reported complexes, only slightly deviating elemental analyses could be obtained. Experimental procedure for X-ray analysis is given below in the crystallographic appendix.

$[PhC(N\textit{t}Bu)_2Si(C_5Me_5)]$[1] was synthesized according to the literature known methods. $[Ni(cod)_2]$ was used as received without further purification.

Synthesis of $[PhC(N\textit{t}Bu)_2SiNi(C_5Me_5)]_2$

Onto a mixture of 100 mg $[PhC(N\textit{t}Bu)_2Si(C_5Me_5)]$ (0.254 mmol, 1.00 eq.) and 70 mg $[Ni(cod)_2]$ (0.254 mmol, 1.00 eq.) THF was condensed at –88 °C. Afterwards the mixture was stirred until it reached ambient temperature, and everything was dissolved. During this process, the colour of the solution changed from yellow to deep green and ended up dark red almost black. After reaching room temperature the mixture was no longer stirred and X-ray suitable crystals formed overnight. The product was isolated as deep red crystals in 45% yield (52 mg, 0.057 mmol).

NMR measurements were not possible due to the insolubility of the product in common organic solvents.

EI-MS (70 eV): m/z (%) = 904 ($[M]^+$, 1), 453 ($1/2[MH]^+$, 1), 384 ($1/2[M]^+$ –N*t*Bu, 6), 328 ($1/2[M]^+$ –N*t*Bu –*t*Bu, 44), 231 ($[PhC(\textit{t}BuN)_2]^+$, 26), 175 ($[PhC(NH)(N\textit{t}Bu)]^+$, 32), 161 ($[PhC(NH)\textit{t}Bu]^+$,44), 119 ($[PhC(NH)2]^+$, 100).

IR (ATR, cm^{-1}): 2952 (s), 2923 (s), 2895 (s), 2852 (s), 1411 (vs), 1389 (m), 1356 (m), 1263 (m), 1203 (w), 787 (w), 744 (m), 706 (m), 602 (w), 502 (m), 423 (w), 374 (w), 308 (w).

RAMAN (excitation wavelength 532 nm, cm^{-1}): 2528, 2425, 1600, 1512, 1068, 751, 625, 465, 357, 297, 201, 128, 98.

Elemental analysis (calcd for $C_{50}H_{76}N_4Si_2Ni_2$): C 65.03 (66.23), H: 8.12 (8.45), N: 5.92 (6.18), due to the formation of silicon carbide carbon values were always too low.

Mass Spectrum

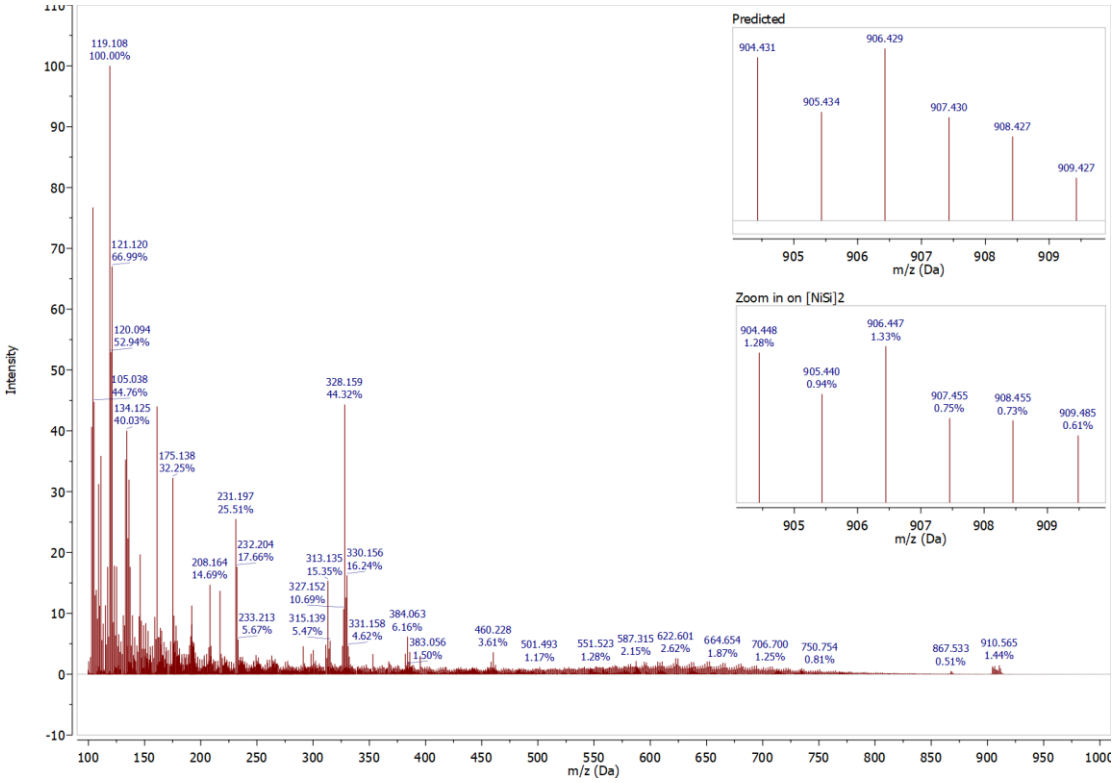

Figure S 1: EI mass spectrum of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$. The signals between 500 and 800 Da are residual noise from measurements prior to this spectrum. The inset shows the simulated and the measured [M]$^+$ peak.

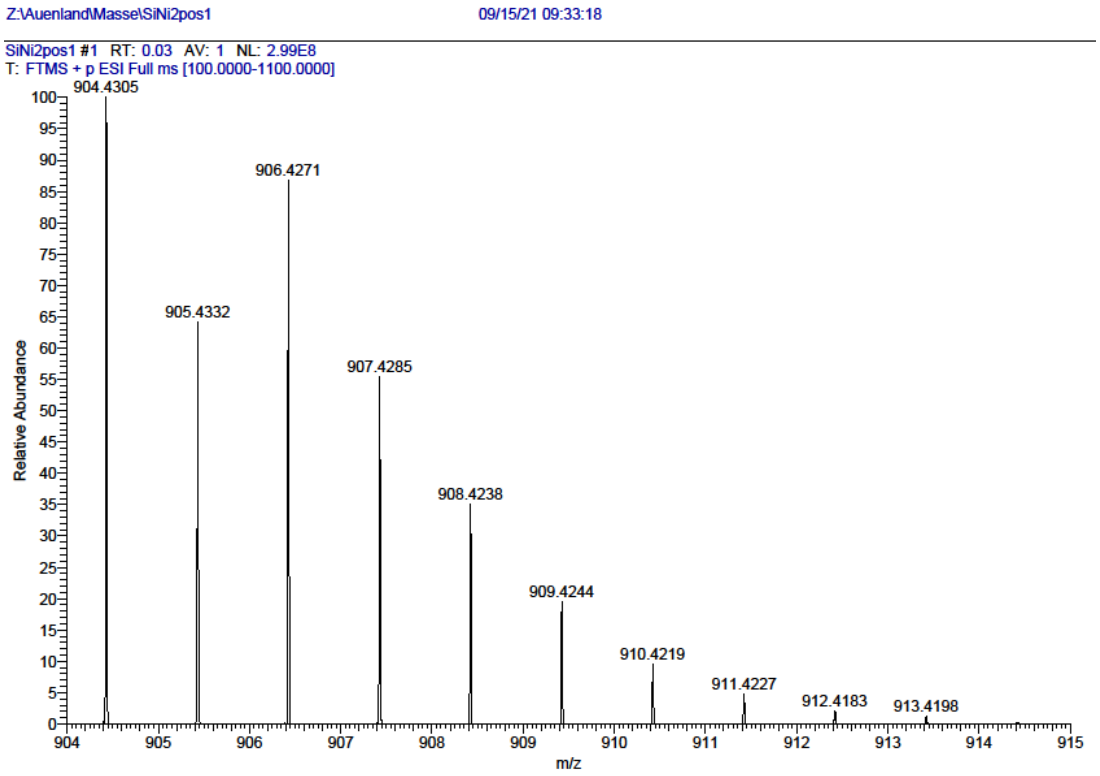

Figure S 2: ESI mass spectrum of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$.

IR Spectra

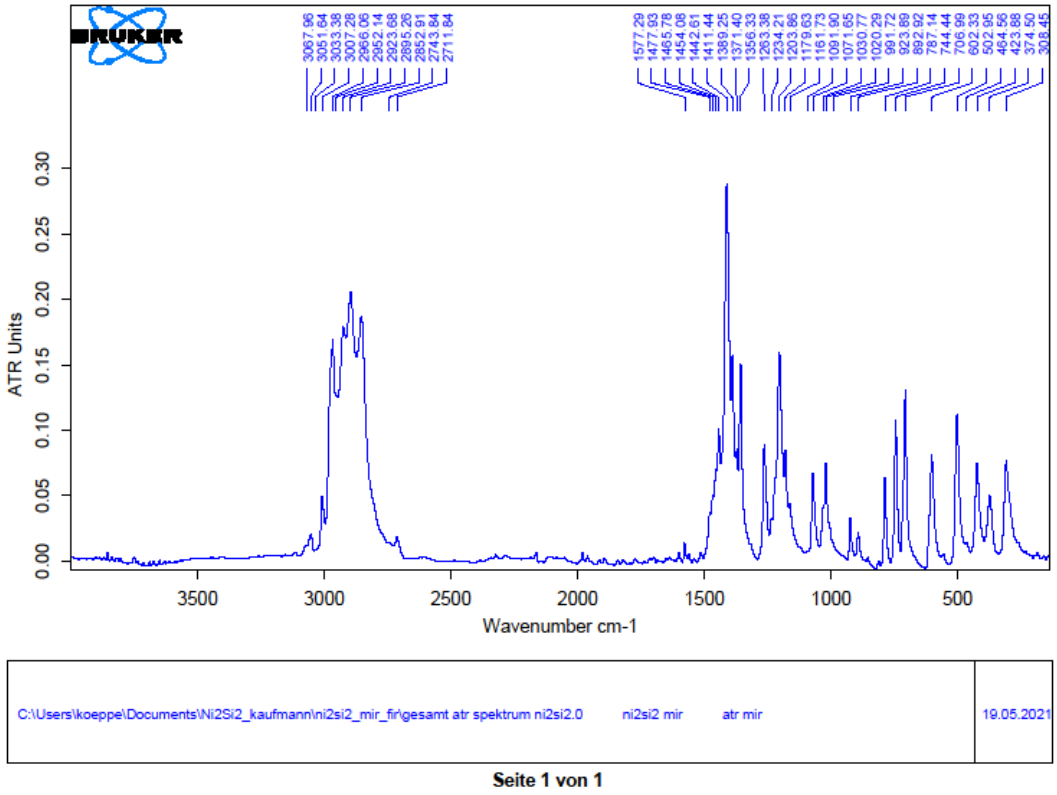

Figure S 3: ATR-IR spectrum of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$.

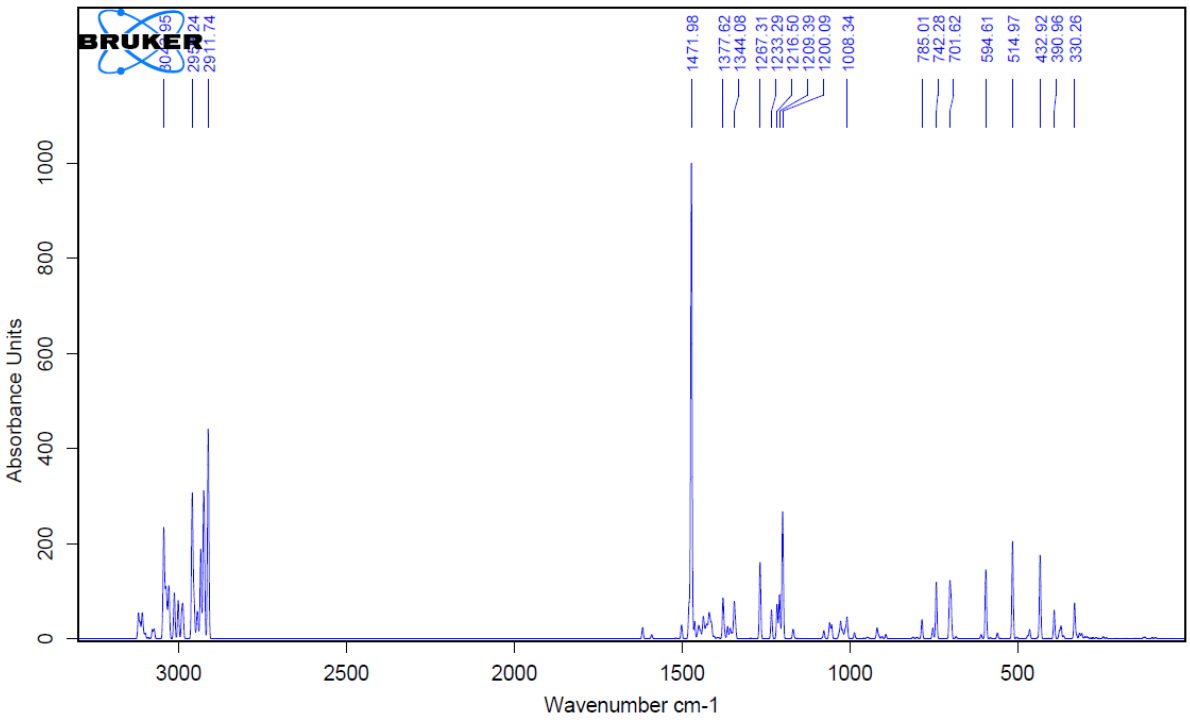

Figure S 4: Theoretical IR spectrum of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$.

RAMAN Spectra

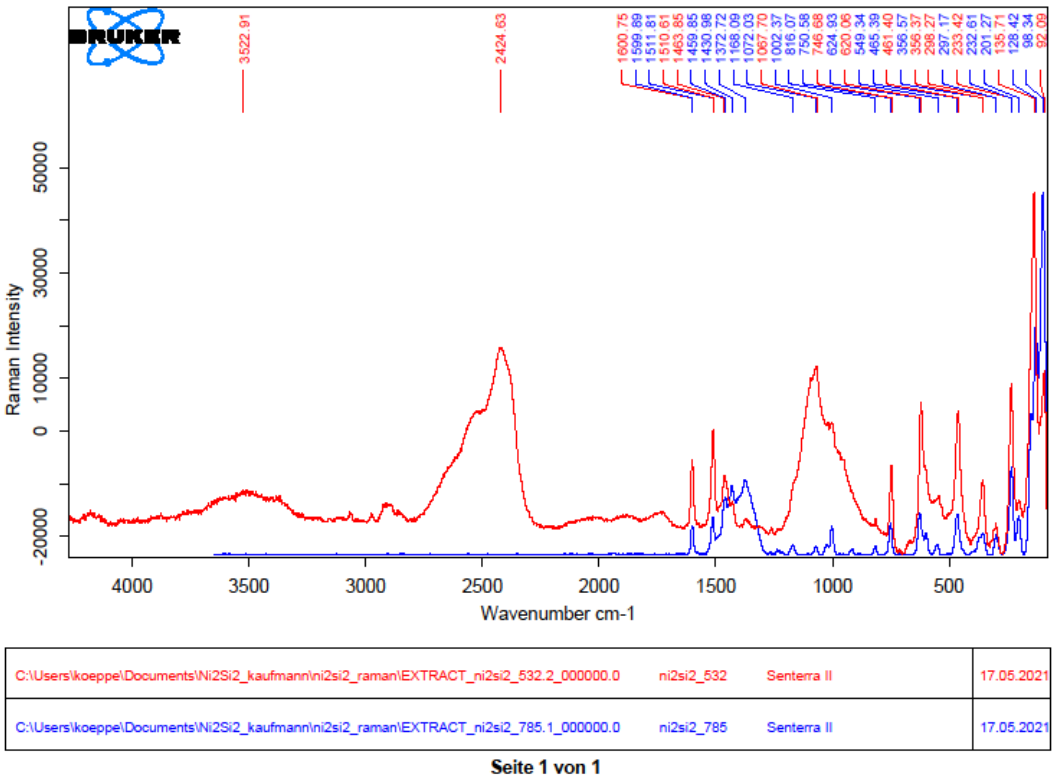

Figure S 5: Raman spectra of of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$ (excitation wavelengths 532 (blue) and 785 (red) nm).

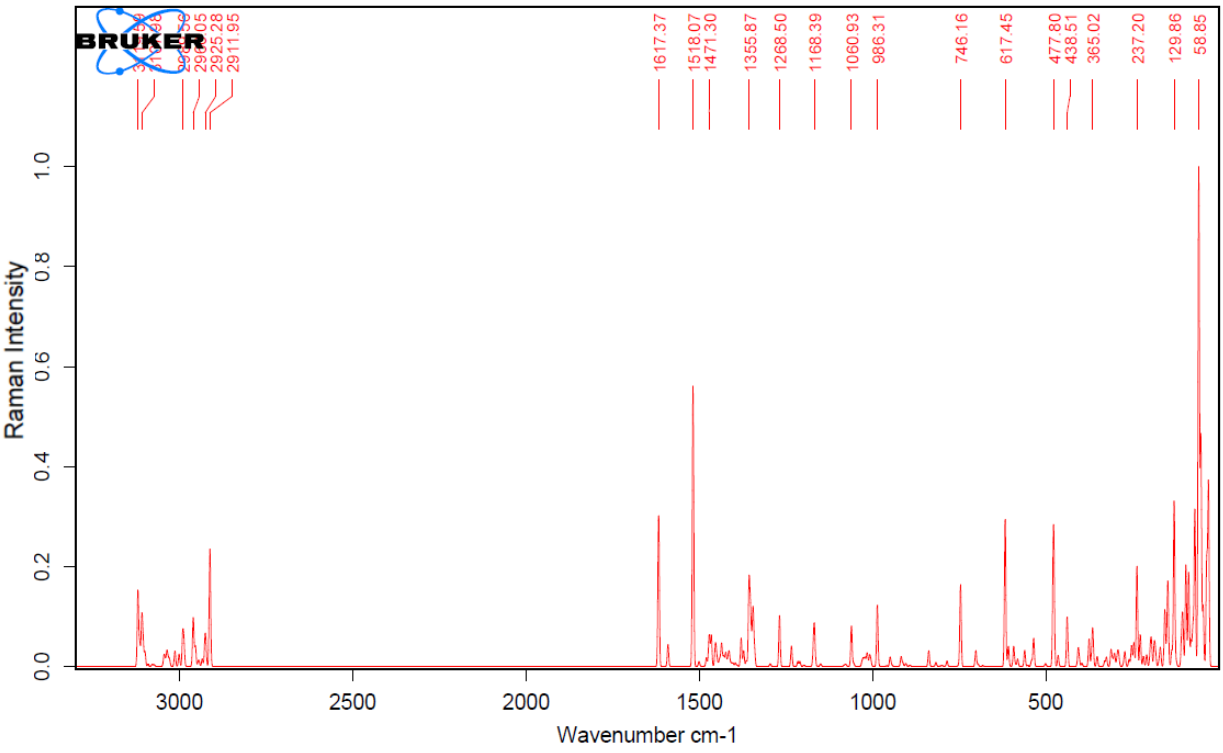

Figure S 6: Theoretical Raman spectrum of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$

Crystallographic Appendix

A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fiber or a mylar loop. The crystal was transferred directly to the cold stream of a STOE IPDS 2 diffractometer. All structures were solved by using the program SHELXS/T[2, 3] using Olex2.[4] The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F^2 by using the program SHELXL.[2, 5] In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance.

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. 2105223. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Compound	**[PhC(N*t*Bu)$_2$SiNi(C$_5$Me$_5$)]$_2$**
Formula	$C_{50}H_{76}N_4Ni_2Si_2$
$D_{calc.}$/ g cm^{-3}	1.249
μ/mm^{-1}	0.868
Formula Weight	906.74
Colour	red
Shape	plate
Size/mm^3	0.21×0.14×0.04
T/K	150
Crystal System	triclinic
Space Group	P-1
a/Å	10.265(2)
b/Å	11.626(2)
c/Å	12.091(2)
α/°	83.66(3)
β/°	68.19(3)
γ/°	64.34(3)
V/Å^3	1205.2(6)
Z	1
Z'	0.5
Wavelength/Å	0.71073
Radiation type	MoK$_\alpha$
Θ_{min}/°	1.947
Θ_{max}/°	27.716
Measured Refl.	11352
Independent Refl.	4741
Reflections with I > 2(I)	3263
R_{int}	0.0774
Parameters	273
Restraints	0
Largest Peak	0.914
Deepest Hole	-0.351
GooF	0.892
wR_2 (all data)	0.1133
wR_2	0.1068
R_1 (all data)	0.0714
R_1	0.0464

Ortep Plots

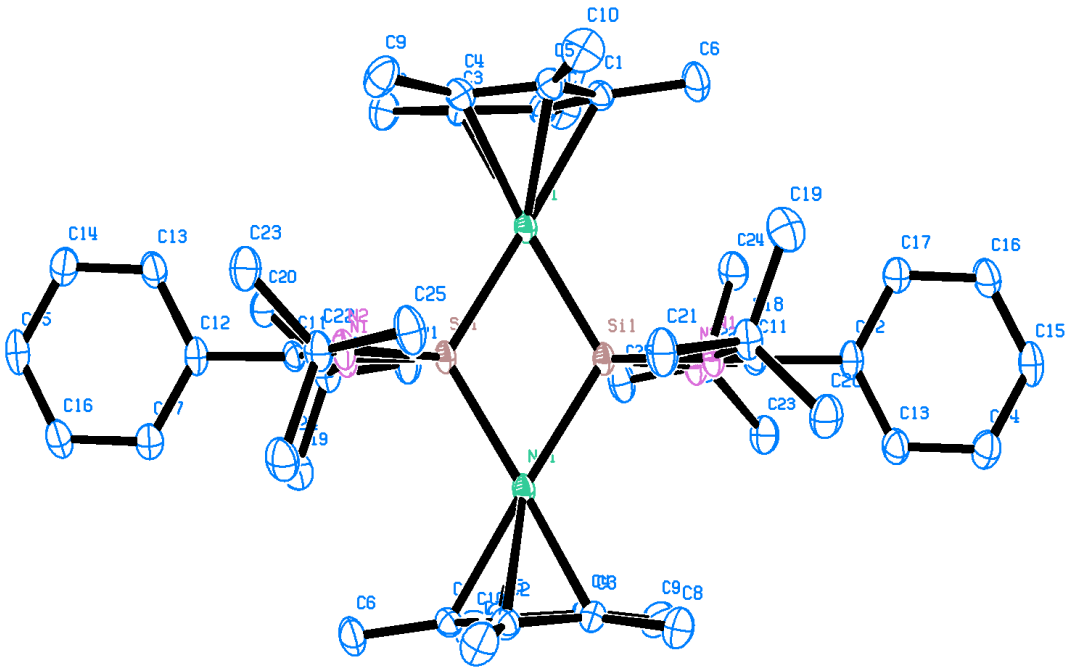

Figure S 7: Ortep plot of the solid-state structure of [PhC(NtBu)$_2$SiNi(C$_5$Me$_5$)]$_2$. Ellipsoids are displayed at 50% probability.

Quantum Chemical Calculations

Table S 1: Coordinates of the molecule Ni2Si2 (given in atomic units).

1.17168905193077	-2.25222166276087	2.29800468649534	ni
0.67308944797225	-1.39979583103823	-1.71758429493157	si
-0.67308944797225	1.39979583103823	1.71758429493157	si
4.16339191502129	-3.19697464763585	4.94362483368674	c
1.60468189864437	-6.19434829954309	2.95744241330451	c
0.18100627448540	-5.16217817293085	5.01248565431217	c
1.73123563634372	-3.24167004283548	6.20742153626859	c
4.05583551510032	-4.97981904213929	2.91159204118965	c
-1.17168905193077	2.25222166276087	-2.29800468649534	ni
3.39620592522497	-2.39882527412535	-3.92606819411147	n
-0.27127683839053	-4.21808674841843	-3.81925584741967	n
-3.39620592522497	2.39882527412535	3.92606819411147	n
0.27127683839053	4.21808674841843	3.81925584741967	n
6.51233378263779	-1.77730378026554	5.69829427278720	c
0.88892896795074	-8.40654708011629	1.34017278551968	c
-2.35399464319454	-6.14735378618860	5.85532573093956	c
1.02895457217020	-1.74530275260845	8.52687708187992	c
6.19955743604441	-5.77074697032933	1.23819903092903	c
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-1.97604839554925	4.20913485573324	5.00801043796624	c
-5.84521446290651	1.29706338663978	4.65827439193746	c

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2.57655759694879	4.79159362285858	8.53710938962272	h
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5.61392706863125	-11.79394905037564	-7.68687870216997	h
-2.95388933364779	6.63651082680101	13.50278480908517	h
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-5.61392706863125	11.79394905037564	7.68687870216997	h
4.98904374735600	-10.74576671454267	-12.27732999724776	h
-4.98904374735600	10.74576671454267	12.27732999724776	h

Table S 2: Vibrational Frequencies, IR intensities and Raman cross sections of $[PhC(NtBu)_2SiNi(C_5Me_5)]_2$.

ν/cm^{-1}		IR intensity/ km·mol^{-1}	Raman cross scattering/%
-9.42	a_g	0	0
30.31	a_u	0.08931	8.72E-17
30.86	a_g	0	25.9375166
35.93	a_g	0	17.4086381
36.28	a_u	0.22785	1.28E-17
46.28	a_g	0	9.45148736
52.78	a_g	0	35.0323569
58.88	a_g	0	100
60.82	a_u	0.00887	0
63.68	a_u	0.00887	0
70.11	a_g	0	23.5769397
73.48	a_u	0.07613	3.09E-18
75.66	a_g	0	6.37397486
80.28	a_u	0.15677	0
81.02	a_g	0	4.87201372
84.92	a_u	0.11666	0
87.98	a_g	0	14.7563557
88.68	a_u	0.71372	1.51E-17
89.72	a_u	0.74217	0
95.99	a_g	0	15.4357375
98.77	a_u	1.04191	1.50E-19
101.89	a_u	0.01971	1.15E-18
104.9	a_g	0	6.44145784
108.27	a_g	0	4.21850225
108.77	a_u	0.23306	2.61E-19
120.16	a_u	1.84043	0
123.85	a_g	0	0.78317439
124.7	a_u	1.34578	1.88E-19
129.86	a_g	0	31.0505193
136.8	a_g	0	2.32704403
140.41	a_u	0.31054	0
147.46	a_g	0	9.99347551
148.99	a_u	0.31567	2.27E-16
149.01	a_g	0	6.24515405
152.5	a_u	0.15417	2.24E-18
153.94	a_g	0	1.35428758
155.4	a_u	0.17795	3.53E-19
156.93	a_g	0	8.32517772
166.96	a_u	0.12606	0
169.64	a_g	0	2.67310771
173.67	a_g	0	0.98442467
174.83	a_u	0.26563	5.49E-19
180.58	a_u	0.28667	1.99E-19
183.46	a_g	0	2.76900259
185.4	a_u	0.06089	0
187.08	a_g	0	4.34614713
189.89	a_u	0.20356	0
195.54	a_g	0	4.71732253
197.08	a_u	0.02124	0
198.82	a_g	0	2.30978446
201.39	a_u	0.16808	7.52E-20
206.25	a_u	0.33023	0
209.16	a_g	0	1.73934649
218.39	a_g	0	1.47461138
224.06	a_u	0.07656	1.09E-20
227.63	a_g	0	4.51145959
235.5	a_u	0.9348	0
237.2	a_g	0	16.1105674
244.74	a_u	2.37692	0
246	a_g	0	3.33378853
252.69	a_g	0	3.59620972
259.4	a_u	0.53303	1.82E-20
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266.07	a_u	1.23813	0
271.94	a_g	0	2.07296811
275.06	a_u	0.73273	0
275.29	a_g	0	0.98047963
281.15	a_u	0.73994	0
289.06	a_u	0.69615	0

289.6	a_g	0	1.63666158
292.93	a_u	2.02458	6.82E-18
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311.89	a_g	0	2.36691171
315.57	a_u	6.69282	0
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325.18	a_g	0	1.55491575
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330.52	a_g	0	0.67651789
334.1	a_u	0.96162	0
351.95	a_g	0	1.44540289
362.55	a_g	0	0.42730121
362.82	a_u	3.26184	1.87E-18
364.22	a_u	0.13008	0
364.62	a_g	0	6.16606353
367.42	a_g	0	2.22466259
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375.53	a_u	9.19962	2.04E-19
390.96	a_u	35.04438	0
396.18	a_g	0	0.49880131
403.5	a_g	0	0.69092109
404.33	a_u	0.31107	4.96E-19
405.38	a_g	0	0.75925757
407.05	a_g	0	2.19788182
410.54	a_u	0.44788	0
432.92	a_u	103.27167	0
438.51	a_g	0	8.67237939
440.18	a_u	1.33673	6.48E-20
464.04	a_u	11.04175	0

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469.86	a_u	3.47402	0
477.11	a_g	0	19.824218
479.19	a_g	0	10.7531617
500.95	a_g	0	0.51679298
501.88	a_u	1.79928	3.99E-21
514.97	a_u	120.14595	0
533.81	a_u	0.16134	9.51E-19
535.27	a_g	0	5.28650871
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592.79	a_g	0	3.31425298
593.09	a_u	4.59525	5.70E-20
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617.45	a_g	0	25.05102
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696	a_g	0	0.33632246
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912.75	a_u	1.93829	0
915.43	a_g	0	0.22840431
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1444.4	a_g	0	0.23971444
1444.86	a_u	9.71496	0
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1449.8	a_u	13.5063	4.36E-21
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1472	a_u	575.89812	0
1472.1	a_g	0	3.6054654
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1517.8	a_u	0.56556	6.89E-21
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2953.78	a_g	0	1.5627679
2953.79	a_u	22.28584	7.74E-21
2958.38	a_u	109.04958	1.70E-22
2958.46	a_g	0	3.10000683
2960.36	a_u	94.54597	0
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3001.52	a_g	0	0.60158484
3001.52	a_u	17.73553	4.50E-20
3012.14	a_g	0	0.76147666
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3028.01	a_g	0	0.45075525
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3031.51	a_g	0	0.83743011
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3114.48	a_u	18.9859	2.75E-18
3119.62	a_u	31.6032	0
3119.65	a_g	0	10.9296644

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