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Highly asymmetric coordination of trimethylsilyl groups to tetrazole and triazole rings: an experimental and computational study in gaseous and crystalline phases

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Supplementary data

Table S1 Details of the GED experiments for **1** and **2**.[a]

	1		**2**	
nozzle-to-film distance / mm	99.4	261.7	97.6	262.1
T_{sample} / K	396	386	393[b]	351[b]
T_{nozzle} / K	415	404	414	371
Δs / nm^{-1}	2	1	2	1
s_{min} / nm^{-1}	100	20	100	40
sw_1 / nm^{-1}	120	40	110	50
sw_2 / nm^{-1}	326	129	310	129
s_{max} / nm^{-1}	370	150	360	140
correlation parameter	0.488	0.492	0.471	0.423
scale factor	0.621(12)	0.753(5)	0.629(14)	0.853(11)
λ / pm	6.13	6.13	6.13	6.13

[a] Numbers in parentheses are the estimated standard deviations of the last digits. [b] This temperature difference was necessary because the beam strength changed between the two experiments for **2**.

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Table S2 Experimental data and refinement statistics for the X-ray crystal structure of 1-trimethylsilyltetrazole, **1**.

M_r	142.25
Cell setting, space group	Monoclinic, $P2_1$
a, b, c/Å	5.916(1), 10.577(1), 6.624(1)
β	105.35(1)°
V/Å^3	399.7(1)
Z	2
D/Mg m^{-3}	1.182
Radiation type	Mo $K\alpha$
Number of reflections for cell parameters	100
θ range/°	3.2–27.1
μ/mm^{-1}	0.220
Temperature/K	133(2)
Crystal form, colour	Colourless
Crystal size/mm	1.0 × 0.25 × 0.25
Data collection	
Diffractometer	Nonius CAD-4 diffractometer
Data collection method	ω scans
Absorption correction	none
Number of measured, independent and observed reflections	2397, 1628, 1430
Criterion for observed reflections	$I > 2\sigma(I)$
R_{int}	0.0937
θ_{max}/°	27.11
Range of *h, k, l*	$-7 \le h \le 7$ $-13 \le k \le 13$ $-6 \le l \le 3$
Refinement	
Refinement on	F^2
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.0471, 0.1194, 1.03
Number of reflections	1628
Number of parameters	106
H-atom treatment	C(51) isotropic, others grouped, same C–H distances, conformation free, Si–C–H fixed (AFIX 138)
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0814\,P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	0.000
$\Delta\sigma_{max}$, $\Delta\sigma_{min}$/e Å^3	0.289, –0.277
Extinction method	none
Extinction coefficient	none
Absolute structure	Flack H D (1983)
Flack parameter	0.3(2)

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Table S3 Calculated coordinates [MP2/6-311++G(3df,3pd)] for **1**.[a]

Atom	*x*	*y*	*z*
N(1)	-0.0535	0.6439	0.0000
N(2)	1.1276	1.3014	0.0000
N(3)	0.8493	2.5884	0.0000
N(4)	-0.4860	2.7849	0.0000
C(5)	-1.0263	1.5778	0.0000
H(51)	-2.0789	1.3581	0.0000
Si(6)	-0.0408	-1.1637	0.0000
C(7)	-1.8384	-1.6428	0.0000
H(71)	-1.9296	-2.7295	0.0000
H(72)	-2.3524	-1.2689	0.8851
H(73)	-2.3524	-1.2689	-0.8851
C(8)	0.8493	-1.6679	-1.5462
H(81)	0.9249	-2.7535	-1.6130
H(82)	0.3289	-1.3069	-2.4326
H(83)	1.8560	-1.2519	-1.5491
C(9)	0.8493	-1.6679	1.5462
H(91)	0.9249	-2.7535	1.6130
H(92)	1.8560	-1.2519	1.5491
H(93)	0.3289	-1.3069	2.4326

Energy (not zero-point corrected) = –665.79350 Hartrees

[a] Coordinates in Å.

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Table S4 Calculated coordinates [MP2/6-311++G(3df,3pd)] for **2**.[a]

Atom	*x*	*y*	*z*
N(1)	-0.0389	0.6367	0.0000
N(2)	1.1656	1.2680	0.0000
C(3)	0.8251	2.5574	0.0000
H(31)	1.5698	3.3352	0.0000
N(4)	-0.5090	2.7979	0.0000
C(5)	-1.0185	1.5746	0.0000
H(51)	-2.0664	1.3251	0.0000
Si(6)	-0.0556	-1.1577	0.0000
C(7)	-1.8589	-1.6235	0.0000
H(71)	-1.9589	-2.7095	0.0000
H(72)	-2.3700	-1.2450	0.8847
H(73)	-2.3700	-1.2450	-0.8847
C(8)	0.8251	-1.6982	-1.5423
H(81)	0.8844	-2.7856	-1.5966
H(82)	0.3094	-1.3393	-2.4323
H(83)	1.8377	-1.2969	-1.5505
C(9)	0.8251	-1.6982	1.5423
H(93)	0.3094	-1.3393	2.4323
H(91)	0.8844	-2.7856	1.5966
H(92)	1.8377	-1.2969	1.5505

Energy (not zero-point corrected) = –649.79269 Hartrees

[a] Coordinates in Å.

Table S5 Calculated coordinates [MP2/6-311++G**] for tetrazole.[a]

Atom	*x*	*y*	*z*
C(1)	1.0715	0.2364	0.0000
H(2)	2.0997	0.5626	0.0000
N(3)	0.0000	1.0555	0.0000
N(4)	-1.1227	0.3171	0.0000
N(5)	-0.7222	-0.9363	0.0000
N(6)	0.6347	-1.0144	0.0000
H(7)	-0.0572	2.0652	0.0000

Energy (not zero-point corrected) = –257.65435 Hartrees

[a] Coordinates in Å.

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Table S6 Calculated coordinates [MP2/6-311++G**] for 1-silyltetrazole.

Atom	*x*	*y*	*z*
C(1)	-1.2759	-0.2997	0.0000
H(2)	-2.1537	0.3288	0.0000
N(3)	0.0000	0.1639	0.0000
N(4)	0.8182	-0.9214	0.0000
N(5)	0.0428	-1.9832	0.0000
N(6)	-1.2658	-1.6241	0.0000
Si(7)	0.7180	1.8146	0.0000
H(8)	-0.4497	2.7086	0.0000
H(9)	1.5205	1.9552	1.2189
H(10)	1.5205	1.9552	-1.2189

Energy (not zero-point corrected) = –547.87986 Hartrees

[a] Coordinates in Å.

Table S7 Calculated coordinates [MP2/6-311++G**] for trimethylsilylpentazole.[a]

Atom	*x*	*y*	*z*
N(1)	-0.0141	0.6627	0.0000
N(2)	1.0360	1.4891	0.0000
N(3)	0.5169	2.7062	0.0000
N(4)	-0.8197	2.6155	0.0000
Si(5)	0.0650	-1.1779	0.0000
N(6)	-1.1658	1.3379	0.0000
C(7)	-0.8197	-1.6791	1.5574
H(8)	-1.8471	-1.3036	1.5560
H(9)	-0.8543	-2.7699	1.6495
H(10)	-0.3099	-1.2814	2.4401
C(11)	-0.8197	-1.6791	-1.5574
H(12)	-0.3099	-1.2814	-2.4401
H(13)	-0.8543	-2.7699	-1.6495
H(14)	-1.8471	-1.3036	-1.5560
C(15)	1.8823	-1.5638	0.0000
H(16)	2.3743	-1.1500	0.8843
H(17)	2.0342	-2.6488	0.0000
H(18)	2.3743	-1.1500	-0.8843

Energy (not zero-point corrected) = –681.53028 Hartrees

[a] Coordinates in Å.

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Table S8 Calculated coordinates [MP2/6-311++G**] for 1-tert-butyltetrazole.[a]

Atom	*x*	*y*	*z*
C(1)	1.0866	1.2098	0.0000
H(2)	2.1275	0.9318	0.0000
N(3)	0.0496	0.3410	0.0000
N(4)	-1.0921	1.0516	0.0000
N(5)	-0.7395	2.3264	0.0000
N(6)	0.6075	2.4499	0.0000
C(7)	0.0025	-1.1375	0.0000
C(8)	1.4328	-1.6699	0.0000
C(9)	-0.7395	-1.5773	1.2626
C(10)	-0.7395	-1.5773	-1.2626
H(11)	1.9789	-1.3505	-0.8930
H(12)	1.9789	-1.3505	0.8930
H(13)	1.3948	-2.7629	0.0000
H(14)	-1.7550	-1.1751	1.2667
H(15)	-0.7869	-2.6703	1.2938
H(16)	-0.2162	-1.2228	2.1562
H(17)	-0.7869	-2.6703	-1.2938
H(18)	-1.7550	-1.1751	-1.2667
H(19)	-0.2162	-1.2228	-2.1562

Energy (not zero-point corrected) = –414.45415 Hartrees

[a] Coordinates in Å.

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Table S9 Interatomic distances (r_a), amplitudes of vibration (u_{h1}) and perpendicular distance corrections (k_{h1}) for the GED refinement of **1**.[a]

	Atom pair	r_a	u(expt.)	k_{h1}	u(calc.)
u_4	C(2)–H(6)	1.066(5)	0.070(4)	0.003	0.074
u_{18}	C(16)–H(18)	1.076(3)	0.072(tied to u_4)	0.004	0.076
u_{14}	C(12)–H(13)	1.076(3)	0.072(tied to u_4)	0.004	0.076
u_{11}	C(8)–H(9)	1.076(3)	0.072(tied to u_4)	0.004	0.076
u_{12}	C(8)–H(10)	1.076(3)	0.072(tied to u_4)	0.004	0.076
u_{13}	C(8)–H(11)	1.076(3)	0.072(tied to u_4)	0.004	0.076
u_{17}	C(16)–H(17)	1.076(3)	0.072(tied to u_4)	0.004	0.076
u_{15}	C(12)–H(14)	1.076(3)	0.071(tied to u_4)	0.004	0.076
u_{19}	C(16)–H(19)	1.076(3)	0.071(tied to u_4)	0.004	0.076
u_{16}	C(12)–H(15)	1.076(3)	0.071(tied to u_4)	0.004	0.076
u_7	N(4)–N(5)	1.292(4)	0.041(2)	-0.001	0.046
u_1	N(1)–C(2)	1.301(4)	0.039(tied to u_7)	0.001	0.043
u_3	C(2)–N(3)	1.335(4)	0.040(tied to u_7)	0.004	0.044
u_2	N(1)–N(5)	1.340(4)	0.043(tied to u_7)	-0.001	0.048
u_5	N(3)–N(4)	1.347(4)	0.042(tied to u_7)	0.003	0.047
u_{133}	H(10)...H(11)	1.712(9)	0.123(fixed)	-0.002	0.123
u_{169}	H(17)...H(18)	1.723(9)	0.124(fixed)	-0.002	0.124
u_{154}	H(13)...H(14)	1.723(9)	0.123(fixed)	-0.002	0.123
u_{124}	H(9)...H(11)	1.725(9)	0.124(fixed)	-0.002	0.124
u_{123}	H(9)...H(10)	1.725(9)	0.124(fixed)	-0.002	0.124
u_{170}	H(17)...H(19)	1.726(9)	0.124(fixed)	-0.002	0.124
u_{160}	H(14)...H(15)	1.726(9)	0.123(fixed)	-0.002	0.123
u_{171}	H(18)...H(19)	1.727(9)	0.124(fixed)	-0.002	0.124
u_{155}	H(13)...H(15)	1.727(9)	0.124(fixed)	-0.002	0.124
u_6	N(3)–Si(7)	1.785(3)	0.044(2)	0.001	0.052
u_{10}	Si(7)–C(16)	1.847(4)	0.045(tied to u_6)	0.001	0.053
u_9	Si(7)–C(12)	1.847(4)	0.045(tied to u_6)	0.001	0.053
u_8	Si(7)–C(8)	1.852(4)	0.045(tied to u_6)	0.002	0.053
u_{22}	N(1)...H(6)	2.102(13)	0.183(tied to u_{51})	-0.001	0.095
u_{52}	N(3)...H(6)	2.103(12)	0.185(tied to u_{51})	-0.007	0.096
u_{51}	N(3)...N(5)	2.107(5)	0.092(7)	0.002	0.048
u_{37}	C(2)...N(5)	2.110(5)	0.093(tied to u_{51})	0.000	0.048
u_{20}	N(1)...N(3)	2.144(5)	0.064(3)	0.002	0.048
u_{36}	C(2)...N(4)	2.159(5)	0.065(tied to u_{20})	-0.004	0.049
u_{21}	N(1)...N(4)	2.166(5)	0.065(tied to u_{20})	-0.003	0.049
u_{106}	Si(7)...H(9)	2.437(7)	0.124(6)	-0.003	0.125
u_{114}	Si(7)...H(19)	2.439(7)	0.123(tied to u_{106})	-0.004	0.124
u_{111}	Si(7)...H(15)	2.439(7)	0.123(tied to u_{106})	-0.004	0.124
u_{113}	Si(7)...H(18)	2.448(7)	0.124(tied to u_{106})	-0.003	0.125
u_{109}	Si(7)...H(13)	2.448(7)	0.124(tied to u_{106})	-0.003	0.125
u_{112}	Si(7)...H(17)	2.449(7)	0.122(tied to u_{106})	-0.004	0.123
u_{110}	Si(7)...H(14)	2.449(7)	0.122(tied to u_{106})	-0.004	0.123
u_{107}	Si(7)...H(10)	2.464(7)	0.123(tied to u_{106})	-0.004	0.124

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u_{108}	Si(7)...H(11)	2.464(7)	0.123(tied to u_{106})	-0.004	0.124
u_{66}	N(4)...Si(7)	2.720(5)	0.057(7)	-0.012	0.089
u_{97}	H(6)...H(11)	2.764(27)	0.498(fixed)	0.192	0.498
u_{96}	H(6)...H(10)	2.764(27)	0.498(fixed)	0.192	0.498
u_{38}	C(2)...Si(7)	2.838(5)	0.051(tied to u_{66})	-0.003	0.080
u_{53}	N(3)...C(8)	2.884(8)	0.104(10)	-0.003	0.106
u_{61}	N(3)...C(16)	2.901(10)	0.110(tied to u_{53})	-0.004	0.112
u_{57}	N(3)...C(12)	2.901(10)	0.110(tied to u_{53})	-0.004	0.112
u_{94}	H(6)...C(8)	3.000(27)	0.284(fixed)	0.140	0.284
u_{119}	C(8)...C(16)	3.067(20)	0.095(tied to u_{150})	-0.003	0.115
u_{115}	C(8)...C(12)	3.067(20)	0.095(tied to u_{150})	-0.003	0.115
u_{150}	C(12)...C(16)	3.075(40)	0.095(6)	-0.002	0.114
u_{64}	N(3)...H(19)	3.106(14)	0.224(tied to u_{150})	0.004	0.269
u_{60}	N(3)...H(15)	3.106(14)	0.224(tied to u_{150})	0.004	0.269
u_{55}	N(3)...H(10)	3.108(12)	0.208(tied to u_{150})	0.004	0.250
u_{56}	N(3)...H(11)	3.108(12)	0.208(tied to u_{150})	0.004	0.250
u_{62}	N(3)...H(17)	3.117(14)	0.222(tied to u_{150})	0.004	0.266
u_{59}	N(3)...H(14)	3.117(14)	0.222(tied to u_{150})	0.004	0.266
u_{93}	H(6)...Si(7)	3.134(21)	0.133(tied to u_{150})	0.000	0.160
u_{74}	N(4)...H(15)	3.136(22)	0.473(tied to u_{75})	0.064	0.445
u_{78}	N(4)...H(19)	3.136(22)	0.473(tied to u_{75})	0.064	0.445
u_{144}	H(11)...H(14)	3.140(46)	0.356(fixed)	0.066	0.356
u_{139}	H(10)...H(17)	3.140(46)	0.355(fixed)	0.066	0.355
u_{79}	N(5)...H(6)	3.144(9)	0.072(tied to u_{150})	-0.009	0.087
u_{168}	H(15)...H(19)	3.144(87)	0.354(fixed)	0.069	0.354
u_{65}	N(4)...H(6)	3.174(8)	0.093(tied to u_{75})	-0.015	0.088
u_{42}	C(2)...H(11)	3.236(16)	0.388(tied to u_{75})	0.095	0.365
u_{41}	C(2)...H(10)	3.236(16)	0.388(tied to u_{75})	0.095	0.365
u_{126}	H(9)...H(13)	3.247(27)	0.388(fixed)	0.052	0.388
u_{131}	H(9)...H(18)	3.247(27)	0.387(fixed)	0.052	0.387
u_{117}	C(8)...H(14)	3.256(30)	0.260(tied to u_{75})	0.010	0.245
u_{120}	C(8)...H(17)	3.256(30)	0.260(tied to u_{75})	0.010	0.245
u_{158}	H(13)...H(18)	3.266(51)	0.386(fixed)	0.062	0.386
u_{165}	H(15)...C(16)	3.268(59)	0.260(tied to u_{75})	0.008	0.245
u_{153}	C(12)...H(19)	3.268(59)	0.260(tied to u_{75})	0.008	0.245
u_{142}	H(11)...C(12)	3.272(30)	0.256(tied to u_{75})	0.007	0.241
u_{138}	H(10)...C(16)	3.272(30)	0.256(tied to u_{75})	0.007	0.241
u_{39}	C(2)...C(8)	3.294(13)	0.199(tied to u_{75})	0.065	0.187
u_{125}	H(9)...C(12)	3.304(21)	0.270(tied to u_{75})	0.003	0.254
u_{129}	H(9)...C(16)	3.304(21)	0.270(tied to u_{75})	0.003	0.254
u_{121}	C(8)...H(18)	3.324(21)	0.282(tied to u_{75})	0.002	0.266
u_{116}	C(8)...H(13)	3.324(21)	0.282(tied to u_{75})	0.002	0.266
u_{152}	C(12)...H(18)	3.324(42)	0.278(tied to u_{75})	0.005	0.262
u_{156}	H(13)...C(16)	3.325(42)	0.278(tied to u_{75})	0.005	0.262
u_{75}	N(4)...C(16)	3.353(17)	0.320(13)	-0.003	0.302
u_{71}	N(4)...C(12)	3.353(17)	0.320(tied to u_{75})	-0.003	0.302

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u_{127}	H(9)...H(14)	3.547(30)	0.403(fixed)	-0.008	0.403
u_{130}	H(9)...H(17)	3.547(30)	0.403(fixed)	-0.008	0.403
u_{159}	H(13)...H(19)	3.567(59)	0.416(fixed)	-0.011	0.416
u_{167}	H(15)...H(18)	3.567(59)	0.416(fixed)	-0.011	0.416
u_{76}	N(4)...H(17)	3.570(22)	0.490(fixed)	-0.028	0.490
u_{73}	N(4)...H(14)	3.570(22)	0.490(fixed)	-0.028	0.490
u_{143}	H(11)...H(13)	3.581(29)	0.408(fixed)	-0.013	0.408
u_{140}	H(10)...H(18)	3.581(29)	0.408(fixed)	-0.013	0.408
u_{80}	N(5)...Si(7)	3.794(4)	0.078(3)	-0.022	0.073
u_{54}	N(3)...H(9)	3.799(8)	0.131(tied to u_{80})	-0.036	0.122
u_{58}	N(3)...H(13)	3.817(9)	0.134(tied to u_{80})	-0.041	0.125
u_{63}	N(3)...H(18)	3.817(9)	0.133(tied to u_{80})	-0.041	0.124
u_{23}	N(1)...Si(7)	3.881(4)	0.071(tied to u_{80})	-0.017	0.066
u_{48}	C(2)...H(17)	3.902(23)	0.453(tied to u_{80})	-0.011	0.421
u_{45}	C(2)...H(14)	3.902(23)	0.453(tied to u_{80})	-0.011	0.421
u_{47}	C(2)...C(16)	3.945(15)	0.245(tied to u_{80})	-0.043	0.228
u_{43}	C(2)...C(12)	3.945(15)	0.245(tied to u_{80})	-0.043	0.228
u_{118}	C(8)...H(15)	3.958(16)	0.137(tied to u_{80})	-0.038	0.127
u_{122}	C(8)...H(19)	3.958(16)	0.136(tied to u_{80})	-0.038	0.127
u_{161}	H(14)...C(16)	3.969(31)	0.136(tied to u_{80})	-0.038	0.127
u_{151}	C(12)...H(17)	3.969(31)	0.135(tied to u_{80})	-0.038	0.126
u_{146}	H(11)...C(16)	3.974(16)	0.135(tied to u_{80})	-0.034	0.126
u_{134}	H(10)...C(12)	3.974(16)	0.135(tied to u_{80})	-0.034	0.126
u_{95}	H(6)...H(9)	4.006(27)	0.307(fixed)	0.077	0.307
u_{67}	N(4)...C(8)	4.119(7)	0.075(7)	-0.055	0.110
u_{100}	H(6)...H(14)	4.157(36)	0.598(fixed)	-0.025	0.598
u_{103}	H(6)...H(17)	4.157(36)	0.598(fixed)	-0.025	0.598
u_{147}	H(11)...H(17)	4.203(29)	0.244(fixed)	-0.032	0.244
u_{136}	H(10)...H(14)	4.203(29)	0.244(fixed)	-0.032	0.244
u_{164}	H(14)...H(19)	4.204(56)	0.245(fixed)	-0.039	0.245
u_{145}	H(11)...H(15)	4.204(29)	0.245(fixed)	-0.039	0.245
u_{141}	H(10)...H(19)	4.204(29)	0.244(fixed)	-0.039	0.244
u_{166}	H(15)...H(17)	4.204(56)	0.244(fixed)	-0.039	0.244
u_{50}	C(2)...H(19)	4.234(17)	0.235(tied to u_{67})	-0.074	0.344
u_{46}	C(2)...H(15)	4.234(17)	0.235(tied to u_{67})	-0.074	0.344
u_{128}	H(9)...H(15)	4.255(18)	0.245(fixed)	-0.045	0.245
u_{132}	H(9)...H(19)	4.255(18)	0.245(fixed)	-0.045	0.245
u_{163}	H(14)...H(18)	4.274(35)	0.252(fixed)	-0.043	0.252
u_{157}	H(13)...H(17)	4.274(35)	0.252(fixed)	-0.043	0.252
u_{135}	H(10)...H(13)	4.287(18)	0.254(fixed)	-0.040	0.254
u_{148}	H(11)...H(18)	4.287(18)	0.254(fixed)	-0.040	0.254
u_{92}	N(5)...H(19)	4.302(20)	0.286(tied to u_{67})	0.005	0.418
u_{88}	N(5)...H(15)	4.302(20)	0.286(tied to u_{67})	0.005	0.418
u_{40}	C(2)...H(9)	4.316(12)	0.134(tied to u_{67})	0.011	0.196
u_{102}	H(6)...C(16)	4.318(27)	0.252(tied to u_{67})	-0.064	0.369
u_{98}	H(6)...C(12)	4.318(27)	0.252(tied to u_{67})	-0.064	0.369

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u_{72}	N(4)...H(13)	4.332(15)	0.199(tied to u_{67})	-0.052	0.290
u_{77}	N(4)...H(18)	4.332(15)	0.199(tied to u_{67})	-0.052	0.290
u_{69}	N(4)...H(10)	4.353(12)	0.188(tied to u_{67})	-0.056	0.275
u_{70}	N(4)...H(11)	4.353(12)	0.188(tied to u_{67})	-0.056	0.275
u_{27}	N(1)...H(11)	4.463(17)	0.444(tied to u_{89})	0.053	0.362
u_{26}	N(1)...H(10)	4.463(17)	0.444(tied to u_{89})	0.053	0.362
u_{89}	N(5)...C(16)	4.474(15)	0.296(14)	-0.030	0.241
u_{85}	N(5)...C(12)	4.474(15)	0.296(tied to u_{89})	-0.030	0.241
u_{90}	N(5)...H(17)	4.507(19)	0.551(tied to u_{89})	-0.028	0.450
u_{87}	N(5)...H(14)	4.507(19)	0.551(tied to u_{89})	-0.028	0.450
u_{24}	N(1)...C(8)	4.548(13)	0.220(tied to u_{89})	0.025	0.179
u_{30}	N(1)...H(14)	4.723(19)	0.422(fixed)	-0.020	0.422
u_{33}	N(1)...H(17)	4.723(19)	0.422(fixed)	-0.020	0.422
u_{105}	H(6)...H(19)	4.770(26)	0.412(fixed)	-0.121	0.412
u_{101}	H(6)...H(15)	4.770(26)	0.412(fixed)	-0.121	0.412
u_{162}	H(14)...H(17)	4.780(21)	0.155(fixed)	-0.063	0.155
u_{137}	H(10)...H(15)	4.781(13)	0.158(fixed)	-0.061	0.158
u_{149}	H(11)...H(19)	4.781(13)	0.158(fixed)	-0.061	0.158
u_{32}	N(1)...C(16)	4.794(14)	0.218(10)	-0.050	0.211
u_{28}	N(1)...C(12)	4.794(14)	0.218(tied to u_{32})	-0.050	0.211
u_{35}	N(1)...H(19)	4.838(19)	0.393(tied to u_{32})	-0.062	0.380
u_{31}	N(1)...H(15)	4.838(19)	0.393(tied to u_{32})	-0.062	0.380
u_{44}	C(2)...H(13)	4.853(13)	0.233(tied to u_{32})	-0.081	0.225
u_{49}	C(2)...H(18)	4.853(13)	0.232(tied to u_{32})	-0.081	0.224
u_{81}	N(5)...C(8)	4.920(10)	0.135(tied to u_{32})	-0.033	0.130
u_{68}	N(4)...H(9)	4.959(8)	0.145(tied to u_{32})	-0.090	0.141
u_{83}	N(5)...H(10)	4.993(14)	0.324(tied to u_{32})	-0.022	0.313
u_{84}	N(5)...H(11)	4.993(14)	0.324(tied to u_{32})	-0.022	0.313
u_{99}	H(6)...H(13)	5.104(26)	0.376(fixed)	-0.091	0.376
u_{104}	H(6)...H(18)	5.104(26)	0.376(fixed)	-0.091	0.376
u_{86}	N(5)...H(13)	5.469(14)	0.251(tied to u_{32})	-0.089	0.243
u_{91}	N(5)...H(18)	5.469(14)	0.250(tied to u_{32})	-0.089	0.241
u_{25}	N(1)...H(9)	5.558(12)	0.190(tied to u_{32})	-0.030	0.184
u_{29}	N(1)...H(13)	5.766(12)	0.212(tied to u_{32})	-0.103	0.205
u_{34}	N(1)...H(18)	5.766(12)	0.211(tied to u_{32})	-0.103	0.204
u_{82}	N(5)...H(9)	5.855(9)	0.144(tied to u_{32})	-0.081	0.139

[a] Distances in Å. Figures in parentheses represent the estimated standard deviations on the last digit. Amplitudes of vibration and distance corrections are derived from a force field calculated at the RHF/6-31G* level.

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Table S10 Interatomic distances (r_a), amplitudes of vibration (u_{h1}) and perpendicular distance corrections (k_{h1}) for the GED refinement of **2**.[a]

	Atom pair	r_a	u(expt.)	k_{h1}	u(calc.)
u_4	C(2)–H(6)	1.063(5)	0.070(3)	0.003	0.074
u_8	C(5)–H(20)	1.063(5)	0.070(tied to u_4)	0.003	0.074
u_{15}	C(12)–H(13)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{19}	C(16)–H(18)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{17}	C(12)–H(15)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{20}	C(16)–H(19)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{12}	C(8)–H(9)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{14}	C(8)–H(11)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{16}	C(12)–H(14)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{18}	C(16)–H(17)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_{13}	C(8)–H(10)	1.075(2)	0.072(tied to u_4)	0.004	0.076
u_1	N(1)–C(2)	1.325(4)	0.043(tied to u_5)	0.001	0.043
u_7	N(4)–C(5)	1.330(4)	0.044(tied to u_5)	-0.001	0.044
u_2	N(1)–C(5)	1.352(4)	0.045(tied to u_5)	-0.001	0.045
u_3	C(2)–N(3)	1.357(4)	0.045(tied to u_5)	0.003	0.045
u_5	N(3)–N(4)	1.357(4)	0.046(2)	0.003	0.046
u_{142}	H(10)...H(11)	1.714(7)	0.123(fixed)	-0.002	0.123
u_{166}	H(13)...H(14)	1.723(7)	0.124(fixed)	-0.002	0.124
u_{185}	H(17)...H(18)	1.723(7)	0.123(fixed)	-0.002	0.123
u_{132}	H(9)...H(11)	1.727(7)	0.124(fixed)	-0.002	0.124
u_{131}	H(9)...H(10)	1.727(7)	0.124(fixed)	-0.002	0.124
u_{167}	H(13)...H(15)	1.728(7)	0.124(fixed)	-0.002	0.124
u_{188}	H(18)...H(19)	1.728(7)	0.123(fixed)	-0.002	0.123
u_{173}	H(14)...H(15)	1.729(7)	0.123(fixed)	-0.002	0.123
u_{186}	H(17)...H(19)	1.729(7)	0.123(fixed)	-0.002	0.123
u_6	N(3)–Si(7)	1.791(4)	0.049(2)	0.001	0.051
u_{10}	Si(7)–C(12)	1.852(3)	0.051(tied to u_6)	0.001	0.053
u_{11}	Si(7)–C(16)	1.852(3)	0.051(tied to u_6)	0.001	0.053
u_9	Si(7)–C(8)	1.857(4)	0.051(tied to u_6)	0.002	0.053
u_{39}	C(2)...C(5)	2.086(10)	0.074(tied to u_{54})	0.000	0.049
u_{83}	N(4)...H(20)	2.098(11)	0.144(tied to u_{54})	-0.008	0.095
u_{37}	N(1)...H(20)	2.107(14)	0.144(tied to u_{54})	-0.003	0.095
u_{54}	N(3)...C(5)	2.114(11)	0.073(7)	0.003	0.048
u_{55}	N(3)...H(6)	2.115(11)	0.145(tied to u_{54})	-0.007	0.096
u_{23}	N(1)...H(6)	2.116(15)	0.142(tied to u_{54})	-0.002	0.094
u_{38}	C(2)...N(4)	2.188(13)	0.060(tied to u_{21})	-0.003	0.050
u_{21}	N(1)...N(3)	2.217(11)	0.059(7)	0.002	0.048
u_{22}	N(1)...N(4)	2.254(9)	0.060(tied to u_{21})	-0.004	0.049
u_{117}	Si(7)...H(15)	2.440(6)	0.094(tied to u_{120})	-0.004	0.124
u_{120}	Si(7)...H(19)	2.440(6)	0.094(6)	-0.004	0.124
u_{112}	Si(7)...H(9)	2.441(6)	0.095(tied to u_{120})	-0.003	0.125
u_{116}	Si(7)...H(14)	2.451(6)	0.094(tied to u_{120})	-0.004	0.123
u_{118}	Si(7)...H(17)	2.451(6)	0.094(tied to u_{120})	-0.004	0.123

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u_{115}	Si(7)...H(13)	2.454(6)	0.095(tied to u_{120})	-0.003	0.125
u_{119}	Si(7)...H(18)	2.454(6)	0.095(tied to u_{120})	-0.003	0.125
u_{114}	Si(7)...H(11)	2.468(6)	0.094(tied to u_{120})	-0.004	0.123
u_{113}	Si(7)...H(10)	2.468(6)	0.094(tied to u_{120})	-0.004	0.123
u_{182}	H(15)...H(19)	2.524(56)	0.354(fixed)	0.068	0.354
u_{70}	N(4)...Si(7)	2.715(12)	0.086(7)	-0.013	0.086
u_{161}	C(12)...C(16)	2.726(29)	0.113(tied to u_{70})	-0.002	0.113
u_{170}	H(13)...H(18)	2.768(36)	0.381(fixed)	0.065	0.381
u_{164}	C(12)...H(19)	2.822(39)	0.208(tied to u_{40})	0.008	0.245
u_{179}	H(15)...C(16)	2.822(39)	0.208(tied to u_{40})	0.008	0.245
u_{40}	C(2)...Si(7)	2.876(7)	0.066(5)	-0.005	0.077
u_{102}	H(6)...H(11)	2.929(32)	0.470(fixed)	0.145	0.470
u_{101}	H(6)...H(10)	2.929(32)	0.470(fixed)	0.145	0.470
u_{168}	H(13)...C(16)	2.938(29)	0.220(tied to u_{40})	0.007	0.260
u_{163}	C(12)...H(18)	2.938(29)	0.220(tied to u_{40})	0.007	0.260
u_{56}	N(3)...C(8)	2.971(9)	0.088(tied to u_{40})	-0.002	0.103
u_{60}	N(3)...C(12)	2.993(9)	0.093(tied to u_{40})	-0.004	0.110
u_{64}	N(3)...C(16)	2.993(9)	0.093(tied to u_{40})	-0.004	0.110
u_{171}	H(13)...H(19)	3.085(38)	0.417(fixed)	-0.011	0.417
u_{181}	H(15)...H(18)	3.085(38)	0.417(fixed)	-0.011	0.417
u_{53}	C(2)...H(20)	3.102(12)	0.074(tied to u_{40})	-0.007	0.087
u_{84}	C(5)...H(6)	3.117(13)	0.073(tied to u_{40})	-0.009	0.087
u_{122}	C(8)...C(12)	3.122(12)	0.097(tied to u_{40})	-0.003	0.114
u_{126}	C(8)...C(16)	3.122(12)	0.097(tied to u_{40})	-0.003	0.114
u_{68}	N(3)...H(20)	3.135(11)	0.074(tied to u_{40})	-0.007	0.087
u_{99}	H(6)...C(8)	3.148(31)	0.226(tied to u_{40})	0.103	0.266
u_{139}	H(9)...H(18)	3.160(23)	0.387(fixed)	0.053	0.387
u_{134}	H(9)...H(13)	3.160(23)	0.387(fixed)	0.053	0.387
u_{98}	H(6)...Si(7)	3.164(21)	0.132(tied to u_{40})	-0.002	0.156
u_{69}	N(4)...H(6)	3.194(13)	0.075(tied to u_{40})	-0.014	0.088
u_{82}	N(4)...H(19)	3.196(27)	0.348(tied to u_{40})	0.047	0.410
u_{78}	N(4)...H(15)	3.196(27)	0.348(tied to u_{40})	0.047	0.410
u_{58}	N(3)...H(10)	3.205(12)	0.209(tied to u_{40})	0.004	0.247
u_{59}	N(3)...H(11)	3.205(12)	0.209(tied to u_{40})	0.004	0.247
u_{63}	N(3)...H(15)	3.206(12)	0.228(tied to u_{40})	0.004	0.268
u_{67}	N(3)...H(19)	3.206(12)	0.228(tied to u_{40})	0.004	0.268
u_{62}	N(3)...H(14)	3.218(12)	0.223(tied to u_{40})	0.003	0.263
u_{65}	N(3)...H(17)	3.218(12)	0.223(tied to u_{40})	0.003	0.263
u_{137}	H(9)...C(16)	3.292(15)	0.245(tied to u_{75})	0.004	0.253
u_{133}	H(9)...C(12)	3.292(15)	0.245(tied to u_{75})	0.004	0.253
u_{123}	C(8)...H(13)	3.316(15)	0.258(tied to u_{75})	0.002	0.266
u_{128}	C(8)...H(18)	3.316(15)	0.258(tied to u_{75})	0.002	0.266
u_{148}	H(10)...H(17)	3.380(29)	0.355(fixed)	0.066	0.355
u_{154}	H(11)...H(14)	3.380(29)	0.354(fixed)	0.066	0.354
u_{75}	N(4)...C(12)	3.384(20)	0.254(14)	-0.009	0.262
u_{79}	N(4)...C(16)	3.384(20)	0.254(tied to u_{75})	-0.009	0.262

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u_{124}	C(8)...H(14)	3.396(18)	0.236(tied to u_{75})	0.011	0.244
u_{127}	C(8)...H(17)	3.396(18)	0.236(tied to u_{75})	0.011	0.244
u_{43}	C(2)...H(10)	3.404(20)	0.345(tied to u_{75})	0.073	0.357
u_{44}	C(2)...H(11)	3.404(20)	0.345(tied to u_{75})	0.073	0.357
u_{152}	H(11)...C(12)	3.413(18)	0.233(tied to u_{75})	0.007	0.240
u_{147}	H(10)...C(16)	3.413(18)	0.233(tied to u_{75})	0.007	0.240
u_{41}	C(2)...C(8)	3.439(17)	0.172(tied to u_{75})	0.046	0.178
u_{77}	N(4)...H(14)	3.587(20)	0.443(fixed)	-0.028	0.443
u_{80}	N(4)...H(17)	3.588(20)	0.443(fixed)	-0.028	0.443
u_{135}	H(9)...H(14)	3.611(19)	0.403(fixed)	-0.007	0.403
u_{138}	H(9)...H(17)	3.611(19)	0.403(fixed)	-0.007	0.403
u_{153}	H(11)...H(13)	3.650(19)	0.407(fixed)	-0.014	0.407
u_{149}	H(10)...H(18)	3.650(19)	0.407(fixed)	-0.014	0.407
u_{162}	C(12)...H(17)	3.685(25)	0.126(fixed)	-0.038	0.126
u_{174}	H(14)...C(16)	3.685(25)	0.125(fixed)	-0.038	0.125
u_{180}	H(15)...H(17)	3.779(40)	0.244(fixed)	-0.040	0.244
u_{177}	H(14)...H(19)	3.779(40)	0.243(fixed)	-0.040	0.243
u_{85}	C(5)...Si(7)	3.807(13)	0.083(9)	-0.022	0.070
u_{57}	N(3)...H(9)	3.865(8)	0.142(tied to u_{85})	-0.035	0.120
u_{66}	N(3)...H(18)	3.888(8)	0.146(tied to u_{85})	-0.040	0.124
u_{61}	N(3)...H(13)	3.888(8)	0.145(tied to u_{85})	-0.040	0.123
u_{169}	H(13)...H(17)	3.923(27)	0.252(fixed)	-0.041	0.252
u_{176}	H(14)...H(18)	3.924(27)	0.251(fixed)	-0.041	0.251
u_{24}	N(1)...Si(7)	3.958(10)	0.073(7)	-0.018	0.066
u_{129}	C(8)...H(19)	3.996(9)	0.141(tied to u_{24})	-0.038	0.127
u_{125}	C(8)...H(15)	3.996(9)	0.140(tied to u_{24})	-0.038	0.126
u_{143}	H(10)...C(12)	4.014(9)	0.139(tied to u_{24})	-0.034	0.125
u_{156}	H(11)...C(16)	4.014(9)	0.139(tied to u_{24})	-0.034	0.125
u_{111}	H(6)...H(20)	4.097(17)	0.116(fixed)	-0.018	0.116
u_{49}	C(2)...C(16)	4.129(11)	0.199(tied to u_{71})	-0.037	0.208
u_{45}	C(2)...C(12)	4.129(11)	0.199(tied to u_{71})	-0.037	0.208
u_{50}	C(2)...H(17)	4.151(17)	0.377(tied to u_{71})	-0.006	0.393
u_{47}	C(2)...H(14)	4.151(17)	0.377(tied to u_{71})	-0.006	0.393
u_{100}	H(6)...H(9)	4.157(31)	0.289(fixed)	0.044	0.289
u_{71}	N(4)...C(8)	4.207(11)	0.099(8)	-0.040	0.103
u_{140}	H(9)...H(19)	4.211(14)	0.244(fixed)	-0.045	0.244
u_{136}	H(9)...H(15)	4.211(14)	0.244(fixed)	-0.045	0.244
u_{158}	H(11)...H(18)	4.247(14)	0.255(fixed)	-0.039	0.255
u_{144}	H(10)...H(13)	4.247(14)	0.255(fixed)	-0.039	0.255
u_{81}	N(4)...H(18)	4.317(20)	0.451(tied to u_{25})	-0.058	0.263
u_{76}	N(4)...H(13)	4.318(20)	0.450(tied to u_{25})	-0.058	0.262
u_{97}	C(5)...H(19)	4.331(29)	0.683(tied to u_{25})	-0.006	0.398
u_{93}	C(5)...H(15)	4.331(29)	0.683(tied to u_{25})	-0.006	0.398
u_{150}	H(10)...H(19)	4.344(17)	0.245(fixed)	-0.040	0.245
u_{155}	H(11)...H(15)	4.344(17)	0.244(fixed)	-0.040	0.244
u_{157}	H(11)...H(17)	4.344(17)	0.243(fixed)	-0.032	0.243

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u_{145}	H(10)...H(14)	4.344(17)	0.242(fixed)	-0.032	0.242
u_{108}	H(6)...H(17)	4.349(27)	0.897(tied to u_{25})	-0.012	0.522
u_{105}	H(6)...H(14)	4.350(27)	0.897(tied to u_{25})	-0.012	0.522
u_{52}	C(2)...H(19)	4.363(15)	0.571(tied to u_{25})	-0.060	0.333
u_{48}	C(2)...H(15)	4.363(15)	0.571(tied to u_{25})	-0.060	0.333
u_{42}	C(2)...H(9)	4.432(16)	0.323(tied to u_{25})	-0.005	0.188
u_{74}	N(4)...H(11)	4.433(14)	0.441(tied to u_{25})	-0.038	0.257
u_{73}	N(4)...H(10)	4.433(14)	0.441(tied to u_{25})	-0.038	0.257
u_{107}	H(6)...C(16)	4.469(22)	0.551(tied to u_{25})	-0.049	0.321
u_{103}	H(6)...C(12)	4.469(22)	0.551(tied to u_{25})	-0.049	0.321
u_{90}	C(5)...C(12)	4.553(21)	0.376(tied to u_{25})	-0.035	0.219
u_{94}	C(5)...C(16)	4.553(21)	0.376(tied to u_{25})	-0.035	0.219
u_{92}	C(5)...H(14)	4.553(23)	0.731(tied to u_{25})	-0.028	0.426
u_{95}	C(5)...H(17)	4.554(23)	0.731(tied to u_{25})	-0.028	0.426
u_{175}	H(14)...H(17)	4.591(20)	0.154(fixed)	-0.063	0.154
u_{27}	N(1)...H(10)	4.625(20)	0.614(tied to u_{25})	0.047	0.357
u_{28}	N(1)...H(11)	4.625(20)	0.614(tied to u_{25})	0.047	0.357
u_{25}	N(1)...C(8)	4.718(17)	0.296(33)	0.019	0.172
u_{121}	Si(7)...H(20)	4.750(14)	0.192(tied to u_{25})	-0.037	0.112
u_{159}	H(11)...H(19)	4.798(9)	0.158(fixed)	-0.061	0.158
u_{146}	H(10)...H(15)	4.798(9)	0.158(fixed)	-0.061	0.158
u_{34}	N(1)...H(17)	4.884(23)	0.777(tied to u_{33})	-0.020	0.420
u_{31}	N(1)...H(14)	4.884(23)	0.776(tied to u_{33})	-0.020	0.420
u_{33}	N(1)...C(16)	4.980(19)	0.388(28)	-0.049	0.210
u_{29}	N(1)...C(12)	4.980(19)	0.388(tied to u_{33})	-0.049	0.210
u_{110}	H(6)...H(19)	4.982(20)	0.378(fixed)	-0.096	0.378
u_{106}	H(6)...H(15)	4.982(20)	0.378(fixed)	-0.096	0.378
u_{51}	C(2)...H(18)	4.984(10)	0.385(tied to u_{33})	-0.076	0.208
u_{46}	C(2)...H(13)	4.984(10)	0.383(tied to u_{33})	-0.076	0.207
u_{32}	N(1)...H(15)	5.003(25)	0.698(tied to u_{33})	-0.058	0.377
u_{36}	N(1)...H(19)	5.003(25)	0.698(tied to u_{33})	-0.058	0.377
u_{72}	N(4)...H(9)	5.007(13)	0.249(tied to u_{33})	-0.074	0.134
u_{86}	C(5)...C(8)	5.022(16)	0.231(tied to u_{33})	-0.022	0.125
u_{190}	H(19)...H(20)	5.027(34)	0.457(fixed)	-0.003	0.457
u_{183}	H(15)...H(20)	5.028(34)	0.457(fixed)	-0.003	0.457
u_{89}	C(5)...H(11)	5.090(19)	0.558(tied to u_{33})	-0.008	0.301
u_{88}	C(5)...H(10)	5.090(19)	0.558(tied to u_{33})	-0.008	0.301
u_{109}	H(6)...H(18)	5.277(22)	0.336(fixed)	-0.078	0.336
u_{104}	H(6)...H(13)	5.278(22)	0.336(fixed)	-0.078	0.336
u_{165}	C(12)...H(20)	5.309(25)	0.530(tied to u_{33})	-0.048	0.286
u_{184}	C(16)...H(20)	5.309(25)	0.530(tied to u_{33})	-0.048	0.286
u_{178}	H(14)...H(20)	5.377(25)	0.501(fixed)	-0.048	0.501
u_{187}	H(17)...H(20)	5.377(25)	0.501(fixed)	-0.048	0.501
u_{96}	C(5)...H(18)	5.534(21)	0.413(tied to u_{33})	-0.092	0.223
u_{91}	C(5)...H(13)	5.535(21)	0.411(tied to u_{33})	-0.092	0.222
u_{26}	N(1)...H(9)	5.713(16)	0.330(tied to u_{33})	-0.035	0.178

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u_{35}	N(1)...H(18)	5.934(17)	0.376(tied to u_{33})	-0.101	0.203
u_{30}	N(1)...H(13)	5.934(17)	0.373(tied to u_{33})	-0.101	0.202
u_{87}	C(5)...H(9)	5.935(15)	0.248(tied to u_{33})	-0.069	0.134
u_{130}	C(8)...H(20)	6.048(16)	0.264(tied to u_{33})	-0.047	0.143
u_{160}	H(11)...H(20)	6.160(20)	0.317(fixed)	-0.034	0.317
u_{151}	H(10)...H(20)	6.160(20)	0.317(fixed)	-0.034	0.317
u_{189}	H(18)...H(20)	6.327(25)	0.300(fixed)	-0.113	0.300
u_{172}	H(13)...H(20)	6.327(25)	0.299(fixed)	-0.113	0.299
u_{141}	H(9)...H(20)	6.947(15)	0.155(fixed)	-0.097	0.155

[a] Distances in Å. Figures in parentheses represent the estimated standard deviations on the last digit. Amplitudes of vibration and distance corrections are derived from a force field calculated at the RHF/6-31G* level.

Table S11 Coordinates of the final refined GED structure of **1**.[a]

Atom	*x*	*y*	*z*
N(1)	0.0000	0.0000	0.0000
N(2)	1.3451	0.0000	0.0000
N(3)	1.7033	1.2442	0.0000
N(4)	0.6289	2.0491	0.0000
C(5)	-0.4108	1.2668	0.0000
H(51)	-1.4345	1.5690	0.0000
Si(6)	-0.9205	-1.5286	0.0000
C(7)	-2.7024	-1.0260	0.0000
H(71)	-3.3390	-1.8949	0.0000
H(72)	-2.9653	-0.4351	0.8614
H(73)	-2.9653	-0.4351	-0.8613
C(8)	-0.4427	-2.4275	-1.5401
H(81)	-0.9548	-3.3713	-1.6250
H(82)	-0.6775	-1.8585	-2.4240
H(83)	0.6151	-2.6302	-1.5579
C(9)	-0.4426	-2.4275	1.5401
H(91)	-0.9547	-3.3713	1.6250
H(92)	0.6151	-2.6301	1.5578
H(93)	-0.6774	-1.8585	2.4240

[a] Coordinates in Å.

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Table S12 Coordinates of the final refined GED structure of **2**.[a]

Atom	*x*	*y*	*z*
N(1)	-1.3170	-1.6529	0.0000
N(2)	0.0000	-1.3321	0.0000
C(3)	0.0000	0.0000	0.0000
H(31)	0.8873	0.5882	0.0000
N(4)	-1.2326	0.5618	0.0000
C(5)	-2.0276	-0.4985	0.0000
H(51)	-3.0918	-0.4710	0.0000
Si(6)	-1.8139	-3.3733	0.0000
C(7)	-3.6678	-3.4783	0.0000
H(71)	-3.9819	-4.5075	0.0000
H(72)	-4.1039	-3.0044	0.8621
H(73)	-4.1039	-3.0044	-0.8622
C(8)	-0.9776	-4.3014	-1.3665
H(81)	-1.2679	-5.3375	-1.3775
H(82)	-1.2234	-3.8890	-2.3294
H(83)	0.0917	-4.2610	-1.2528
C(9)	-0.9776	-4.3014	1.3665
H(91)	-1.2679	-5.3375	1.3775
H(92)	0.0917	-4.2610	1.2529
H(93)	-1.2235	-3.8890	2.3295

[a] Coordinates in Å.

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Table S13 Least-squares correlation matrix (×100) from the GED refinement of **1**.[a]

	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}	p_{12}	p_{13}	p_{14}	p_{15}	p_{16}	p_{17}	p_{18}	p_{19}
p_1	100	7	3	0	6	-2	1	-6	2	10	0	0	-2	0	-1	0	-4	-8	17
p_2		100	2	0	-12	9	-1	-15	10	-1	-2	-17	7	0	-4	0	13	-17	50
p_3			100	0	0	-5	0	-2	-3	0	0	-12	-8	0	0	0	-1	2	-1
p_4				100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_5					100	-6	1	-1	3	15	8	4	1	0	-4	0	12	-9	20
p_6						100	0	-4	-8	-1	0	-1	-9	0	5	0	13	25	-42
p_7							100	-1	6	-2	0	5	1	0	-1	0	4	0	2
p_8								100	-3	-3	-1	2	-3	0	-1	0	4	18	-31
p_9									100	3	1	-8	-5	0	2	0	-3	43	6
p_{10}										100	-47	4	0	0	-3	0	-13	-3	8
p_{11}											100	-2	1	0	-1	0	-15	-1	3
p_{12}												100	-30	0	1	0	1	-5	-6
p_{13}													100	0	3	0	-1	2	0
p_{14}														100	0	0	0	0	0
p_{15}															100	0	-9	-2	6
p_{16}																100	0	0	0
p_{17}																	100	-5	4
p_{18}																		100	-49
p_{19}																			100

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	p_{20}	p_{21}	p_{22}	u_1	u_{11}	u_{25}	u_{31}	u_{33}	u_{36}	u_{45}	u_{49}	u_{55}	u_{88}	u_{98}	u_{114}	u_{142}	u_{154}	k_1	k_2
p_1	-8	0	0	2	15	11	-1	-3	0	4	-7	5	25	8	-8	11	8	-6	21
p_2	-34	1	0	-1	66	-7	-18	-9	13	36	-5	-4	17	10	2	13	17	-5	2
p_3	2	0	0	0	-6	3	0	-5	0	-3	2	6	1	0	1	-3	-6	0	-2
p_4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_5	-13	0	0	4	-14	0	21	0	-40	-11	-9	2	1	0	-2	-14	-10	16	-12
p_6	16	-1	0	-2	4	-70	-1	-4	3	43	3	6	23	-4	-1	16	13	-4	-3
p_7	26	0	0	2	-1	-7	3	-2	5	-3	-1	-5	-5	-22	-9	2	-2	-1	1
p_8	-13	0	0	0	-11	1	5	0	0	25	5	-2	17	2	1	9	7	0	-2
p_9	-19	0	0	0	8	-4	-4	-3	10	-5	10	4	0	6	2	4	-5	1	-1
p_{10}	-6	0	0	1	4	4	9	1	-8	-8	-4	6	8	3	2	0	-13	-17	10
p_{11}	-2	0	0	-2	1	0	1	1	-4	2	1	3	-8	-2	1	-4	9	-4	1
p_{12}	2	2	0	0	-13	0	1	6	-6	28	-36	-10	17	-7	-24	-3	47	3	-3
p_{13}	3	-1	0	0	4	5	0	-17	0	-9	5	5	3	-3	1	-1	-21	1	-3
p_{14}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_{15}	-6	1	0	0	-2	-3	-1	-2	-3	5	6	39	9	3	-12	-5	25	-1	1
p_{16}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_{17}	-9	2	0	1	3	-13	-4	1	4	-19	-22	-5	-13	-16	8	4	-30	10	-5
p_{18}	20	0	0	-1	-11	-21	2	-10	10	7	-30	-7	10	-13	-10	-1	-7	1	0
p_{19}	-63	-1	0	1	34	31	-11	7	-11	-28	-17	10	-20	-4	10	-14	-7	-1	5
p_{20}	100	1	0	0	-21	-12	8	-8	33	7	13	-5	11	21	-4	14	-2	1	-3
p_{21}		100	0	0	1	1	0	-1	1	-6	0	-5	24	3	3	2	-11	0	0
p_{22}			100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
u_1				100	2	9	3	0	-7	0	1	0	1	-1	-1	-1	1	2	1
u_{11}					100	21	1	-1	16	26	2	3	16	19	3	9	15	13	55
u_{25}						100	17	6	-4	-27	1	0	-11	14	2	-13	-5	18	48
u_{31}							100	2	-52	0	8	2	4	6	-1	6	0	9	33
u_{33}								100	-3	-9	0	42	-19	8	22	-2	-3	6	7
u_{36}									100	4	10	1	1	16	8	33	-5	-8	-4
u_{45}										100	17	-8	56	16	-20	17	71	11	3
u_{49}											100	6	8	24	10	34	15	6	8
u_{55}												100	-4	31	2	0	-4	-2	10

u_{88}	100	33	-24	12	35	3	10
u_{98}		100	21	10	10	13	19
u_{114}			100	3	-25	0	3
u_{142}				100	6	-16	1
u_{154}					100	15	5
k_1						100	19
k_2							100

[a] k_1 and k_2 are scale factors.

Table S14 Least-squares correlation matrix (×100) from the GED refinement of **2**.

	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}	p_{11}	p_{12}	p_{13}	p_{14}	p_{15}	p_{16}	p_{17}	p_{18}	p_{19}
p_1	100	5	2	0	1	-3	2	-4	-3	21	-4	-6	0	0	-7	0	-22	9	-5
p_2		100	-1	0	-1	-3	2	-2	0	3	0	-16	-1	0	9	0	18	-27	31
p_3			100	0	-1	-2	0	-2	0	-1	0	-3	-2	0	-4	0	1	4	-5
p_4				100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_5					100	-4	1	-4	-5	5	9	-1	0	0	-10	0	23	-13	18
p_6						100	2	-6	0	1	-1	11	-6	0	14	0	7	12	-24
p_7							100	1	-1	0	1	3	1	0	-4	0	1	-5	2
p_8								100	0	1	-1	8	-4	0	8	0	1	2	-8
p_9									100	2	0	2	-1	0	1	0	-6	33	-6
p_{10}										100	-56	0	0	0	-15	0	-11	-2	5
p_{11}											100	-4	-1	0	11	0	-25	-2	2
p_{12}												100	-12	0	-45	0	7	-6	-46
p_{13}													100	0	12	0	-2	2	-4
p_{14}														100	0	0	0	0	0
p_{15}															100	0	-3	-12	-24
p_{16}																100	0	0	0
p_{17}																	100	-17	-9
p_{18}																		100	-46
p_{19}																			100

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	p_{20}	p_{21}	p_{22}	p_{23}	u_1	u_{16}	u_{26}	u_{33}	u_{37}	u_{40}	u_{49}	u_{54}	u_{88}	u_{107}	u_{113}	u_{124}	u_{153}	u_{159}	k_1	k_2
p_1	18	-2	0	0	-6	2	-1	15	15	-9	-2	21	36	3	2	28	9	10	-32	-5
p_2	-19	-1	0	0	-1	2	59	15	11	2	-2	19	19	6	4	13	10	12	-7	-2
p_3	4	0	0	0	0	1	-5	-2	-1	-7	-3	-1	-1	-1	-4	6	-3	-3	0	0
p_4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_5	-13	0	0	0	-22	20	2	5	10	4	-2	2	-16	-9	14	-9	17	0	47	8
p_6	14	0	0	0	0	-40	-2	2	-16	-10	-8	-3	-2	-7	-16	14	-15	5	-1	-2
p_7	11	0	0	0	0	2	2	11	-10	0	1	1	9	4	-1	-3	-9	4	1	0
p_8	-7	0	0	0	0	-2	-2	7	-6	-6	-3	0	-3	-3	-8	11	-6	3	1	0
p_9	-8	0	0	0	0	-1	0	-3	-4	-3	1	1	1	2	-4	1	-5	0	1	0
p_{10}	-9	0	0	0	2	-2	-8	0	-3	5	0	0	-3	-1	3	2	0	1	-34	-1
p_{11}	0	1	0	0	-4	0	1	-3	-2	1	-2	2	-3	3	-2	-2	-3	-2	-1	-2
p_{12}	37	6	0	1	2	-7	-14	8	1	-39	0	22	2	32	-32	20	-31	34	5	-7
p_{13}	4	1	0	0	0	2	-1	-4	-5	-14	-3	-7	-3	-5	-11	1	-7	-3	1	-1
p_{14}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_{15}	9	-6	0	0	1	-4	7	-15	16	-1	-17	-64	-17	-12	29	37	-5	-5	0	5
p_{16}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_{17}	9	4	0	0	-6	3	18	-8	24	1	-6	-18	2	-5	19	-16	0	-6	43	5
p_{18}	45	-1	0	-1	3	-9	-15	16	11	-18	6	31	18	-19	5	9	-29	1	-1	-5
p_{19}	-85	-3	0	0	-2	16	19	-7	-39	45	12	14	-8	-1	-9	-46	47	-19	2	7
p_{20}	100	2	0	0	-1	-12	-8	46	54	-41	-12	0	48	5	14	43	-19	29	1	-10
p_{21}		100	0	0	0	0	0	0	5	0	0	-7	0	-1	1	14	4	0	0	1
p_{22}			100	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
p_{23}				100	0	0	0	0	1	-1	3	-2	0	-1	1	0	1	0	0	0
u_1					100	36	18	0	-4	3	4	4	-4	6	-2	-2	-5	-1	4	29
u_{16}						100	35	6	14	6	5	8	-2	2	13	-9	12	-5	46	62
u_{26}							100	27	20	1	-2	13	31	0	10	1	16	9	36	53
u_{33}								100	35	-8	-6	22	75	18	5	13	33	52	10	8
u_{37}									100	-2	-12	-13	37	-4	47	23	22	12	17	7
u_{40}										100	33	-24	-7	-19	47	-56	32	-15	-3	4
u_{49}											100	18	-7	6	3	-16	-4	-2	0	1
u_{54}												100	18	40	-39	7	-5	21	2	0

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u_{88}	100	11	8	12	32	43	-4	-4
u_{107}		100	-29	22	-4	64	-6	-4
u_{113}			100	-8	32	-8	14	7
u_{124}				100	-3	22	-13	-7
u_{153}					100	-4	15	4
u_{159}						100	-2	-5
k_1							100	43
k_2								100

[a] k_1 and k_2 are scale factors.

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Table S15 Fractional atomic coordinates for heavy atoms and equivalent isotropic displacement parameters (Å^2) for **1**. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

	a	*b*	*c*	U_{eq}
N(1)	1588(3)	7726(3)	5489(3)	32(1)
N(2)	520(7)	8822(3)	4702(5)	50(1)
N(3)	-1246(7)	8526(3)	3196(5)	55(1)
N(4)	-1455(6)	7270(3)	2904(5)	48(1)
C(5)	333(7)	6808(3)	4324(6)	42(1)
Si(6)	4050(1)	7694(1)	7827(1)	30(1)
C(7)	5632(7)	6218(3)	7616(7)	42(1)
C(8)	5727(8)	9133(4)	7674(8)	49(1)
C(9)	2667(4)	7706(6)	10014(4)	46(1)

Table S16 Anisotropic displacement parameters (× 10^3 Å^2) for **1**.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	40(1)	27(1)	31(1)	6(2)	11(1)	6(1)
N(2)	61(2)	36(1)	45(2)	-1(1)	1(1)	19(1)
N(3)	56(2)	60(2)	42(2)	1(1)	1(2)	22(2)
N(4)	43(1)	61(2)	39(2)	-2(1)	7(1)	-1(1)
C(5)	51(2)	34(1)	39(2)	2(1)	8(2)	-8(1)
Si(6)	34(1)	28(1)	29(1)	-1(1)	11(1)	-2(1)
C(7)	41(2)	34(2)	49(2)	-3(2)	9(2)	8(1)
C(8)	55(3)	44(2)	46(2)	-1(2)	10(2)	-15(2)
C(9)	43(1)	63(2)	34(1)	0(2)	15(1)	-2(2)

Table S17 Hydrogen coordinates (× 10^4) and isotropic displacement parameters /Å^2 × 10^3 for **1**.

	x	*y*	*z*	U_{eq}
H(51)	610(90)	5960(50)	4600(70)	71(12)
H(71)	6920(50)	6154(17)	8730(50)	84(19)
H(72)	6090(60)	6227(15)	6400(50)	80(20)
H(73)	4660(40)	5540(20)	7610(60)	90(20)
H(81)	6990(40)	9194(15)	8860(40)	56(13)
H(82)	4760(30)	9837(18)	7600(50)	51(13)
H(83)	6290(50)	9100(14)	6480(40)	80(20)
H(91)	3840(20)	7780(40)	11300(20)	56(8)
H(92)	1830(60)	6940(20)	10010(40)	68(17)
H(93)	1620(60)	8400(20)	9860(30)	65(17)

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Table S18 Bond lengths and angles for crystalline **1**.

Bond length/Å		Angle/°	
N(1)-C(5)	1.337(4)	C(5)-N(1)-N(2)	105.5(2)
N(1)-N(2)	1.357(4)	C(5)-N(1)-Si(6)	132.4(2)
N(1)-Si(6)	1.8238(18)	N(2)-N(1)-Si(6)	121.9(2)
N(2)-N(3)	1.278(5)	N(3)-N(2)-N(1)	107.0(3)
N(3)-N(4)	1.343(5)	N(2)-N(3)-N(4)	112.3(4)
N(4)-C(5)	1.309(5)	C(5)-N(4)-N(3)	103.9(4)
C(5)-H(51)	0.92(5)	N(4)-C(5)-N(1)	111.3(3)
Si(6)-C(8)	1.835(4)	N(4)-C(5)-H(51)	125(3)
Si(6)-C(9)	1.842(2)	N(1)-C(5)-H(51)	123(3)
Si(6)-C(7)	1.844(4)	N(1)-Si(6)-C(8)	105.04(16)
C(7)-H(71)	0.9152	N(1)-Si(6)-C(9)	104.26(9)
C(7)-H(72)	0.9152	C(8)-Si(6)-C(9)	113.4(2)
C(7)-H(73)	0.9152	N(1)-Si(6)-C(7)	104.97(15)
C(8)-H(81)	0.9320	C(8)-Si(6)-C(7)	113.92(13)
C(8)-H(82)	0.9320	C(9)-Si(6)-C(7)	113.9(2)
C(8)-H(83)	0.9320	Si(6)-C(7)-H(71)	109.5
C(9)-H(91)	0.9506	Si(6)-C(7)-H(72)	109.5
C(9)-H(92)	0.9506	H(71)-C(7)-H(72)	109.5
C(9)-H(93)	0.9506	Si(6)-C(7)-H(73)	109.5
		H(71)-C(7)-H(73)	109.5
		H(72)-C(7)-H(73)	109.5
		Si(6)-C(8)-H(81)	109.5
		Si(6)-C(8)-H(82)	109.5
		H(81)-C(8)-H(82)	109.5
		Si(6)-C(8)-H(83)	109.5
		H(81)-C(8)-H(83)	109.5
		H(82)-C(8)-H(83)	109.5
		Si(6)-C(9)-H(91)	109.5
		Si(6)-C(9)-H(92)	109.5
		H(91)-C(9)-H(92)	109.5
		Si(6)-C(9)-H(93)	109.5
		H(91)-C(9)-H(93)	109.5
		H(92)-C(9)-H(93)	109.5

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Table S19 Torsion angles for crystalline **1**.

Torsion angle/°	
C(5)-N(1)-N(2)-N(3)	0.6(3)
Si(6)-N(1)-N(2)-N(3)	-174.3(3)
N(1)-N(2)-N(3)-N(4)	0.1(6)
N(2)-N(3)-N(4)-C(5)	-0.8(7)
N(3)-N(4)-C(5)-N(1)	1.2(6)
N(2)-N(1)-C(5)-N(4)	-1.2(4)
Si(6)-N(1)-C(5)-N(4)	173.0(2)
C(5)-N(1)-Si(6)-C(8)	150.6(3)
N(2)-N(1)-Si(6)-C(8)	-36.0(3)
C(5)-N(1)-Si(6)-C(9)	-89.9(4)
N(2)-N(1)-Si(6)-C(9)	83.5(3)
C(5)-N(1)-Si(6)-C(7)	30.2(3)
N(2)-N(1)-Si(6)-C(7)	-156.4(3)

Table S20 Calculated coordinates (MP2/6-311+G*) for **1** with C(5)–N(1)–Si(6) angle fixed at the GED-determined value.[a]

Atom	*x*	*y*	*z*
N(1)	-0.0085	0.6501	0.0000
N(2)	1.1550	1.3426	0.0000
N(3)	0.8378	2.6243	0.0000
N(4)	-0.5080	2.7840	0.0000
C(5)	-1.0158	1.5569	0.0000
H(51)	-2.0670	1.3107	0.0000
Si(6)	-0.0401	-1.1720	0.0000
C(7)	-1.8523	-1.6188	0.0000
H(71)	-1.9636	-2.7081	0.0000
H(72)	-2.3715	-1.2442	0.8866
H(73)	-2.3715	-1.2442	-0.8866
C(8)	0.8378	-1.6940	-1.5551
H(81)	0.8939	-2.7842	-1.6361
H(82)	0.3252	-1.3196	-2.4455
H(83)	1.8589	-1.3033	-1.5699
C(9)	0.8378	-1.6940	1.5551
H(91)	0.8939	-2.7842	1.6361
H(92)	1.8589	-1.3033	1.5699
H(93)	0.3252	-1.3196	2.4455

Energy (not zero-point corrected) = –665.44716 Hartrees

[a] Coordinates in Å.

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Table S21 Calculated coordinates (MP2/6-311+G*) for **1** with C(7)–Si(6)–N(1)–C(5) torsion fixed at the value determined using X-ray diffraction.[a]

Atom	*x*	*y*	*z*
N(1)	0.6459	0.0688	-0.0955
N(2)	1.3636	-1.0831	-0.0474
N(3)	2.6361	-0.7435	0.0154
N(4)	2.7718	0.6049	0.0224
C(5)	1.5369	1.0882	-0.0343
H(51)	1.2735	2.1354	-0.0565
Si(6)	-1.1724	-0.0061	0.0100
C(7)	-1.7551	1.6266	-0.6818
H(71)	-2.8491	1.6555	-0.7161
H(72)	-1.4328	2.4790	-0.0771
H(73)	-1.3938	1.7779	-1.7029
C(8)	-1.6670	-1.4571	-1.0404
H(81)	-2.7537	-1.5893	-1.0426
H(82)	-1.3439	-1.3225	-2.0763
H(83)	-1.2129	-2.3791	-0.6702
C(9)	-1.5805	-0.2221	1.8144
H(91)	-2.6615	-0.2976	1.9705
H(92)	-1.1233	-1.1347	2.2071
H(93)	-1.2177	0.6184	2.4129

Energy (not zero-point corrected) = –665.44698 Hartrees

[a] Coordinates in Å.

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Figure S1 Experimental and final weighted difference (experimental minus theoretical) molecular-scattering intensity curves for **1**.

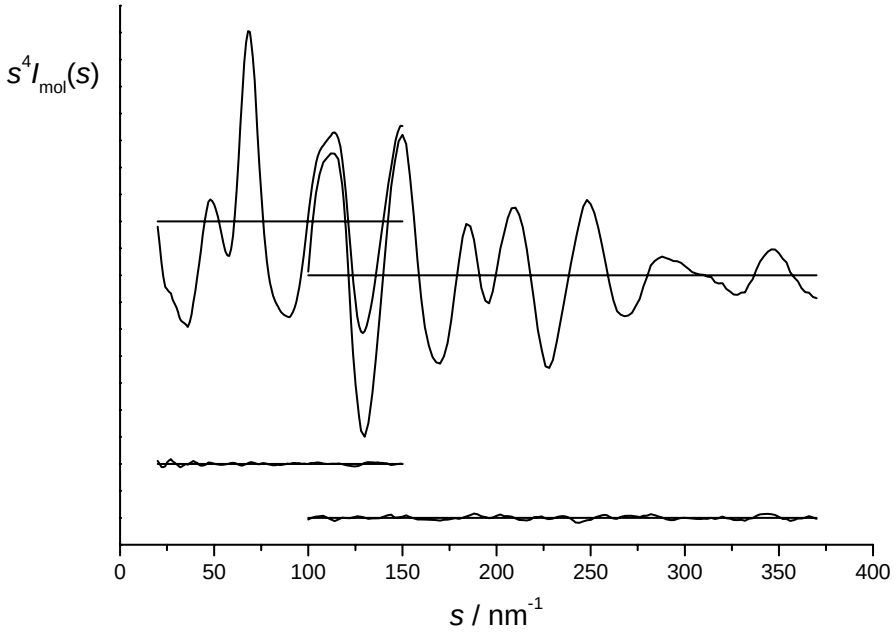

Figure S2 Experimental and final weighted difference (experimental minus theoretical) molecular-scattering intensity curves for **2**.