

Gas Electron Diffraction Then and Now: from trisilyl phosphine to *iso*-propyl(*tert*-butyl)(trichlorosilyl)phosphine

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Supporting Information

Table S1. Nozzle-to-plate distances (mm), weighting functions (nm^{-1}), and electron wavelengths (μm) used in the electron-diffraction study.

Nozzle-to-plate distances ^a	Δs	s_{min}	sw_1	sw_2	s_{max}	Electron wavelength
256.73	2	20	40	104	120	6.020
94.32	4	84	104	256	300	6.020

^a Determined by reference to the scattering pattern of benzene vapour.

Table S2. Calculated coordinates at the B3LYP-D3/Def2TZVP level for conformer +77+.^a

Atom	x	y	z
P(1)	-85.2	27.2	-82.4
Si(2)	119.9	-24.3	-5.8
C(3)	-126.7	193.3	-1.6
C(4)	-206.0	-98.2	-3.8
Cl(5)	243.9	135.5	-48.4
Cl(6)	191.5	-187.2	-110.0
Cl(7)	143.6	-68.2	195.3
C(8)	-95.4	306.3	-100.6
C(9)	-68.7	225.0	136.7
H(10)	-235.5	186.4	7.9
C(11)	-154.7	-240.0	-33.0
C(12)	-339.1	-77.4	-78.6
C(13)	-229.8	-82.1	146.7
H(14)	12.1	315.0	-117.5
H(15)	-130.4	401.8	-60.4
H(16)	-143.3	290.2	-197.2
H(17)	39.0	241.7	131.3
H(18)	-86.7	146.1	209.3
H(19)	-113.7	316.9	175.1
H(20)	-327.8	-94.0	-185.9
H(21)	-379.4	23.0	-63.9
H(22)	-413.4	-148.2	-40.9
H(23)	-138.1	-94.3	204.2
H(24)	-300.7	-158.4	180.2
H(25)	-273.1	15.0	171.0
H(26)	-129.8	-253.7	-138.3
H(27)	-232.5	-312.5	-7.3
H(28)	-66.4	-264.7	26.1

^a Coordinates are given in pm.

Table S3. Calculated coordinates at the B3LYP-D3/Def2TZVP level for conformer +51--.^a

Atom	x	y	z
P(1)	-81.0	30.8	-89.3
Si(2)	118.4	-27.8	-2.0
C(3)	-115.8	204.2	-22.1
C(4)	-208.9	-87.9	-9.7
Cl(5)	264.6	84.0	-95.4
Cl(6)	154.6	-226.3	-46.5
Cl(7)	150.6	-7.1	201.6
C(8)	-23.7	306.0	-90.9
C(9)	-118.7	227.2	129.0
H(10)	-216.7	220.8	-61.2
C(11)	-213.4	-212.0	-100.9
C(12)	-345.8	-18.2	-16.2
C(13)	-180.4	-132.6	134.3
H(14)	78.2	300.1	-52.6
H(15)	-60.4	407.1	-71.6
H(16)	-19.8	291.3	-198.9
H(17)	-20.1	213.6	173.3
H(18)	-187.8	160.5	180.3
H(19)	-150.7	329.8	149.7
H(20)	-368.3	18.2	-116.7
H(21)	-353.4	65.5	53.2
H(22)	-423.5	-90.3	10.9
H(23)	-89.7	-192.8	140.9
H(24)	-263.1	-194.8	169.9
H(25)	-169.9	-48.8	202.9
H(26)	-239.1	-185.3	-203.5
H(27)	-289.4	-281.3	-63.7
H(28)	-118.2	-265.0	-102.5

^a Coordinates are given in pm.

Table S4. Calculated coordinates at the B3LYP-D3/Def2TZVP level for conformer -91(-).^a

Atom	x	y	z
P(1)	78.7	-12.0	-83.6
Si(2)	-132.3	-1.8	-7.1
C(3)	131.5	-179.8	-13.0
C(4)	175.2	130.3	-0.1
Cl(5)	-232.4	-159.6	-95.2
Cl(6)	-221.6	173.7	-68.6
Cl(7)	-167.8	-17.3	196.5
C(8)	159.2	-192.5	137.1
C(9)	248.1	-236.2	-95.7
H(10)	43.8	-241.1	-36.2
C(11)	144.8	256.1	-83.6
C(12)	324.9	97.6	-14.2
C(13)	142.3	158.6	147.0
H(14)	248.6	-137.4	166.4
H(15)	176.7	-297.6	161.9
H(16)	76.0	-157.4	197.8
H(17)	340.5	-181.1	-78.2
H(18)	226.7	-233.3	-202.6
H(19)	266.1	-340.3	-67.6
H(20)	351.9	73.8	-117.3
H(21)	355.2	14.5	49.3
H(22)	383.3	185.0	16.0
H(23)	39.7	193.0	159.9
H(24)	208.0	238.1	183.8
H(25)	156.7	71.5	210.6
H(26)	171.2	242.1	-188.5
H(27)	203.3	339.9	-44.6
H(28)	39.6	284.0	-78.6

^a Coordinates are given in pm.

Table S5. Calculated coordinates at the B3LYP-D3/Def2TZVP level for conformer +143--.^a

Atom	x	y	z
P(1)	87.9	24.0	75.9
Si(2)	-125.1	-10.4	7.2
C(3)	139.8	177.7	-22.9
C(4)	186.5	-121.0	-3.0
Cl(5)	-247.2	123.0	106.5
Cl(6)	-189.3	-199.5	59.7
Cl(7)	-164.8	10.5	-195.3
C(8)	259.9	243.3	47.3
C(9)	29.1	282.6	-38.1
H(10)	169.8	144.1	-122.5
C(11)	170.9	-242.2	90.4
C(12)	335.2	-81.9	-5.6
C(13)	143.1	-158.7	-145.2
H(14)	230.1	282.3	144.9
H(15)	295.9	327.2	-12.7
H(16)	343.5	175.5	63.0
H(17)	-11.8	311.8	58.8
H(18)	-53.1	248.9	-100.9
H(19)	70.8	372.3	-84.6
H(20)	371.5	-51.9	92.9
H(21)	355.7	-1.7	-76.4
H(22)	393.5	-168.9	-37.1
H(23)	43.2	-202.2	-147.5
H(24)	211.9	-233.5	-185.8
H(25)	144.0	-73.0	-212.7
H(26)	205.9	-219.4	191.2
H(27)	230.9	-325.2	51.8
H(28)	67.9	-276.4	97.2

^a Coordinates are given in pm.

Table S6. Calculated coordinates at the B3LYP-D3/Def2TZVP level for conformer +165+-.^a

Atom	x	y	z
P(1)	-82.5	22.6	-79.8
Si(2)	128.3	-12.2	-3.6
C(3)	-129.0	177.5	20.2
C(4)	-190.6	-118.0	-4.1
Cl(5)	254.7	126.3	-90.4
Cl(6)	206.5	-194.9	-58.7
Cl(7)	148.1	5.6	202.0
C(8)	-273.2	219.2	-12.1
C(9)	-34.7	295.0	-8.2
H(10)	-122.4	153.0	126.4
C(11)	-121.8	-254.1	-22.7
C(12)	-320.4	-120.4	-87.4
C(13)	-223.0	-99.2	144.6
H(14)	-286.2	237.2	-119.1
H(15)	-296.4	312.3	40.4
H(16)	-346.8	145.4	19.0
H(17)	-23.8	313.2	-115.3
H(18)	64.6	280.3	33.6
H(19)	-75.9	385.6	36.9
H(20)	-299.3	-142.4	-192.1
H(21)	-375.5	-26.6	-83.4
H(22)	-386.1	-199.0	-48.9
H(23)	-132.5	-93.7	205.2
H(24)	-281.4	-184.9	179.7
H(25)	-282.3	-9.9	163.8
H(26)	-83.5	-267.9	-123.9
H(27)	-194.9	-333.3	-3.7
H(28)	-39.5	-268.4	47.0

^a Coordinates are given in pm.

Table S7. Refined and calculated (B3LYP-D3/Def2TZVP) amplitudes of vibration (u), associated r_a distances and corresponding correction values (k) for the r_{hl} refinement of +77++.^{a,b}

	Atom pair	r_a	u_{GED}	k	$u_{calc.}$
u_1	C(9)-H(18)	108.6(4)	8.3(6)	0.4	7.6
u_2	C(13)-H(23)	108.6(4)	8.3(Tied to u_1)	0.4	7.6
u_3	C(13)-H(25)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_4	C(11)-H(28)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_5	C(8)-H(16)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_6	C(9)-H(17)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_7	C(12)-H(20)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_8	C(11)-H(26)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_9	C(8)-H(14)	108.6(4)	8.3(Tied to u_1)	0.4	7.7
u_{10}	C(12)-H(21)	108.6(4)	8.4(Tied to u_1)	0.4	7.7
u_{11}	C(8)-H(15)	108.6(4)	8.4(Tied to u_1)	0.4	7.7
u_{12}	C(11)-H(27)	108.6(4)	8.4(Tied to u_1)	0.4	7.7
u_{13}	C(9)-H(19)	108.6(4)	8.4(Tied to u_1)	0.4	7.7
u_{14}	C(12)-H(22)	108.6(4)	8.4(Tied to u_1)	0.4	7.7
u_{15}	C(13)-H(24)	108.6(4)	8.4(Tied to u_1)	0.4	7.7
u_{16}	C(3)-H(10)	108.6(4)	8.4(Tied to u_1)	0.4	7.8
u_{17}	C(4)-C(13)	153.1(2)	4.4(3)	0.2	5.3
u_{18}	C(3)-C(9)	153.1(2)	4.4(Tied to u_{17})	0.1	5.3
u_{19}	C(3)-C(8)	153.1(2)	4.4(Tied to u_{17})	0.2	5.3
u_{20}	C(4)-C(11)	153.1(2)	4.4(Tied to u_{17})	0.2	5.3
u_{21}	C(4)-C(12)	153.1(2)	4.5(Tied to u_{17})	0.2	5.3
u_{22}	H(17)...H(19)	175.7(7)	12.4(fixed)	0.0	12.4
u_{23}	H(24)...H(25)	175.7(7)	12.4(fixed)	0.0	12.4
u_{24}	H(27)...H(28)	175.7(7)	12.4(fixed)	0.0	12.4
u_{25}	H(21)...H(22)	175.7(7)	12.4(fixed)	0.0	12.4
u_{26}	H(17)...H(18)	175.7(7)	12.4(fixed)	0.0	12.4
u_{27}	H(14)...H(15)	175.7(7)	12.4(fixed)	-0.1	12.4
u_{28}	H(18)...H(19)	175.7(7)	12.4(fixed)	0.0	12.4
u_{29}	H(23)...H(24)	175.7(7)	12.4(fixed)	0.0	12.4

u_{30}	H(14)...H(16)	175.7(7)	12.4(fixed)	0.0	12.4
u_{31}	H(26)...H(28)	175.7(7)	12.4(fixed)	0.0	12.4
u_{32}	H(26)...H(27)	175.7(7)	12.4(fixed)	0.0	12.4
u_{33}	H(20)...H(21)	175.7(7)	12.4(fixed)	0.0	12.4
u_{34}	H(23)...H(25)	175.7(7)	12.3(fixed)	0.0	12.3
u_{35}	H(20)...H(22)	175.7(7)	12.4(fixed)	0.0	12.4
u_{36}	H(15)...H(16)	175.7(7)	12.4(fixed)	-0.1	12.4
u_{37}	P(1)-C(3)	187.4(5)	5.1(5)	0.2	5.9
u_{38}	P(1)-C(4)	189.1(5)	5.2(Tied to u_{37})	0.2	6.1
u_{39}	Si(2)-Cl(6)	204.0(1)	5.2(Tied to u_{41})	0.2	5.1
u_{40}	Si(2)-Cl(5)	204.0(1)	5.2(Tied to u_{41})	0.2	5.2
u_{41}	Si(2)-Cl(7)	204.0(1)	5.3(2)	0.2	5.3
u_{42}	C(8)...H(10)	215.1(17)	10.8(Tied to u_{43})	0.0	10.8
u_{43}	C(9)...H(10)	213.2(8)	10.8(12)	0.0	10.8
u_{44}	C(4)...H(24)	217.0(5)	11.5(Tied to u_{54})	-0.2	10.8
u_{45}	C(4)...H(20)	217.0(5)	11.5(Tied to u_{54})	-0.2	10.8
u_{46}	C(3)...H(19)	217.0(5)	11.6(Tied to u_{54})	-0.2	10.9
u_{47}	C(4)...H(22)	217.0(5)	11.6(Tied to u_{54})	-0.2	10.9
u_{48}	C(3)...H(15)	217.0(5)	11.6(Tied to u_{54})	-0.2	10.9
u_{49}	C(3)...H(17)	217.0(5)	11.5(Tied to u_{54})	-0.2	10.8
u_{50}	C(3)...H(14)	217.0(5)	11.5(Tied to u_{54})	-0.1	10.8
u_{51}	C(4)...H(25)	217.0(5)	11.5(Tied to u_{54})	-0.1	10.8
u_{52}	C(4)...H(23)	217.0(5)	11.3(Tied to u_{54})	-0.1	10.7
u_{53}	C(3)...H(16)	217.0(5)	11.5(Tied to u_{54})	-0.2	10.8
u_{54}	C(4)...H(20)	217.0(5)	11.5(11)	-0.1	10.8
u_{55}	C(4)...H(26)	217.0(5)	11.5(Tied to u_{54})	-0.2	10.8
u_{56}	C(4)...H(28)	217.0(5)	11.5(Tied to u_{54})	-0.1	10.8
u_{57}	C(3)...H(18)	217.0(5)	11.5(Tied to u_{54})	-0.1	10.8
u_{58}	C(4)...H(21)	217.0(5)	11.5(Tied to u_{54})	-0.1	10.8
u_{59}	P(1)-Si(2)	225.5(6)	6.0(fixed)	0.3	6.0
u_{60}	H(10)...H(21)	382.3(39)	29.7(fixed)	6.8	29.7
u_{61}	H(11)...H(18)	219.3(84)	31.2(fixed)	7.0	31.2

u_{62}	P(1)...H(10)	234.6(9)	11.9(fixed)	0.0	11.9
u_{63}	H(10)...H(25)	234.3(51)	32.0(fixed)	4.3	32.0
u_{64}	H(10)...H(19)	304.3(9)	18.2(fixed)	0.4	18.2
u_{65}	H(18)...H(23)	227.1(73)	33.0(fixed)	8.0	33.0
u_{66}	H(22)...H(27)	379.2(31)	24.3(fixed)	3.0	24.3
u_{67}	H(10)...H(16)	247.3(26)	18.5(fixed)	0.3	18.5
u_{68}	H(22)...H(24)	315.7(38)	24.1(fixed)	2.7	24.1
u_{69}	H(10)...H(15)	251.8(23)	18.7(fixed)	0.2	18.7
u_{70}	C(11)...C(12)	251.6(20)	7.3(Tied to u_{71})	-0.1	7.5
u_{71}	C(12)...C(13)	249.6(9)	7.2(6)	0.0	7.4
u_{72}	C(11)...C(13)	249.6(9)	7.3(Tied to u_{71})	-0.1	7.5
u_{73}	H(15)...H(19)	302.7(40)	24.7(fixed)	3.4	24.7
u_{74}	H(24)...H(27)	375.1(19)	24.7(fixed)	2.4	24.7
u_{75}	C(8)...C(9)	251.6(8)	7.3(Tied to u_{71})	-0.1	7.6
u_{76}	H(10)...H(18)	249.0(19)	18.5(fixed)	0.1	18.5
u_{77}	H(23)...H(28)	250.9(35)	24.4(fixed)	2.3	24.4
u_{78}	H(21)...H(25)	301.7(40)	25.0(fixed)	2.5	25.0
u_{79}	H(20)...H(26)	300.6(49)	25.3(fixed)	2.6	25.3
u_{80}	H(14)...H(17)	320.1(38)	26.8(fixed)	2.8	26.8
u_{81}	C(12)...H(27)	281.8(33)	16.6(fixed)	0.3	16.6
u_{82}	C(13)...H(22)	276.1(22)	16.9(fixed)	0.3	16.9
u_{83}	C(11)...H(24)	272.2(20)	16.5(fixed)	0.2	16.5
u_{84}	C(9)...H(15)	272.6(20)	17.3(fixed)	0.4	17.3
u_{85}	C(13)...H(28)	269.0(21)	17.0(fixed)	0.2	17.0
u_{86}	C(11)...H(20)	274.7(34)	17.3(fixed)	0.2	17.3
u_{87}	C(12)...H(24)	276.8(20)	16.4(fixed)	0.1	16.4
u_{88}	C(12)...H(25)	271.5(22)	16.3(fixed)	0.2	16.3
u_{89}	P(1)...C(12)	271.8(8)	8.1(6)	0.0	8.3
u_{90}	C(11)...H(22)	346.6(16)	17.1(fixed)	0.1	17.1
u_{91}	C(8)...H(17)	278.2(20)	17.9(fixed)	0.1	17.9
u_{92}	C(8)...H(19)	275.0(23)	17.1(fixed)	0.1	17.1
u_{93}	C(13)...H(18)	262.2(60)	23.3(fixed)	6.0	23.3

u_{94}	C(13)...H(27)	344.9(8)	17.2(fixed)	0.0	17.2
u_{95}	C(11)...H(23)	276.1(22)	16.3(fixed)	0.0	16.3
u_{96}	C(13)...H(21)	272.2(20)	17.5(fixed)	0.1	17.5
u_{97}	P(1)...C(8)	277.4(9)	8.2(Tied to u_{89})	-0.2	8.4
u_{98}	C(12)...H(26)	271.7(29)	17.2(fixed)	0.0	17.2
u_{99}	P(1)...C(11)	277.8(8)	8.4(Tied to u_{89})	0.0	8.6
u_{100}	C(9)...H(14)	280.7(23)	18.3(fixed)	-0.1	18.3
u_{101}	Cl(7)...H(23)	282.0(44)	25.5(fixed)	7.2	25.5
u_{102}	C(4)...H(10)	285.5(23)	18.4(fixed)	0.8	18.4
u_{103}	C(3)...H(25)	281.9(35)	23.3(fixed)	2.7	23.3
u_{104}	P(1)...H(26)	375.4(9)	18.5(fixed)	0.5	18.5
u_{105}	P(1)...H(20)	286.1(23)	18.4(fixed)	0.4	18.4
u_{106}	P(1)...C(13)	289.6(8)	7.8(Tied to u_{89})	0.0	8.0
u_{107}	Cl(5)...H(17)	453.7(57)	28.2(fixed)	5.3	28.2
u_{108}	P(1)...H(16)	289.6(22)	18.5(fixed)	0.6	18.5
u_{109}	P(1)...H(21)	372.0(8)	18.7(fixed)	0.3	18.7
u_{110}	C(9)...H(25)	286.8(61)	24.5(fixed)	3.7	24.5
u_{111}	P(1)...C(9)	293.0(9)	7.8(Tied to u_{89})	-0.1	8.0
u_{112}	H(10)...C(12)	297.1(36)	23.6(fixed)	1.8	23.6
u_{113}	H(20)...H(27)	261.2(51)	27.9(fixed)	-0.5	27.9
u_{114}	H(24)...H(28)	297.7(39)	26.5(fixed)	-0.5	26.5
u_{115}	Cl(5)...H(14)	290.1(63)	34.3(fixed)	6.2	34.3
u_{116}	Cl(6)...H(28)	300.0(63)	29.5(fixed)	4.7	29.5
u_{117}	H(15)...H(17)	255.0(32)	29.8(fixed)	-0.7	29.8
u_{118}	H(22)...H(25)	253.3(36)	26.7(fixed)	-0.6	26.7
u_{119}	C(3)...C(4)	299.6(12)	9.4(fixed)	0.2	9.4
u_{120}	H(10)...C(13)	299.2(42)	25.2(fixed)	1.1	25.2
u_{121}	Si(2)...H(28)	296.3(41)	24.4(fixed)	3.0	24.4
u_{122}	P(1)...H(14)	301.3(23)	19.9(fixed)	-0.1	19.9
u_{123}	H(10)...H(14)	305.6(14)	12.7(fixed)	-1.7	12.7
u_{124}	H(10)...H(17)	245.7(16)	12.7(fixed)	-1.6	12.7
u_{125}	Si(2)...H(17)	446.4(23)	26.6(fixed)	2.5	26.6

u_{126}	C(3)...H(21)	446.2(27)	24.5(fixed)	2.7	24.5
u_{127}	P(1)...H(28)	307.1(23)	17.3(fixed)	0.1	17.3
u_{128}	H(21)...H(24)	254.9(32)	26.6(fixed)	-1.0	26.6
u_{129}	Cl(7)...H(18)	312.3(66)	36.7(fixed)	4.5	36.7
u_{130}	P(1)...H(18)	309.3(20)	16.9(fixed)	0.6	16.9
u_{131}	P(1)...H(25)	311.0(21)	17.0(fixed)	0.2	17.0
u_{132}	P(1)...H(23)	309.8(21)	16.7(fixed)	0.2	16.7
u_{133}	H(22)...H(26)	373.7(26)	27.0(fixed)	-1.1	27.0
u_{134}	H(20)...H(23)	372.7(23)	25.6(fixed)	-1.1	25.6
u_{135}	H(14)...H(19)	260.2(38)	28.7(fixed)	-1.4	28.7
u_{136}	P(1)...H(17)	386.6(9)	17.6(fixed)	-0.1	17.6
u_{137}	Si(2)...C(3)	326.5(9)	10.0(10)	0.1	9.9
u_{138}	Cl(6)...H(26)	447.4(39)	37.3(fixed)	3.0	37.3
u_{139}	C(3)...C(13)	324.5(24)	14.3(fixed)	0.6	14.3
u_{140}	Cl(6)...Cl(7)	328.4(11)	10.2(Tied to u_{142})	-0.1	10.1
u_{141}	Cl(5)...Cl(6)	328.4(11)	10.1(Tied to u_{142})	-0.2	10.0
u_{142}	Cl(5)...Cl(7)	323.8(24)	10.3(5)	-0.1	10.3
u_{143}	Cl(7)...H(17)	453.8(47)	40.6(fixed)	2.8	40.6
u_{144}	Cl(7)...H(28)	323.0(85)	43.4(fixed)	3.8	43.4
u_{145}	C(9)...H(23)	317.9(66)	29.1(fixed)	2.4	29.1
u_{146}	Si(2)...C(4)	332.2(9)	9.6(Tied to u_{137})	0.1	9.5
u_{147}	Si(2)...H(23)	334.8(37)	21.8(fixed)	2.4	21.8
u_{148}	H(19)...H(25)	377.4(72)	32.1(fixed)	3.7	32.1
u_{149}	Si(2)...H(18)	340.9(54)	27.4(fixed)	1.0	27.4
u_{150}	Si(2)...C(9)	339.8(24)	14.4(14)	0.6	14.5
u_{151}	C(4)...H(18)	334.4(41)	20.7(fixed)	2.8	20.7
u_{152}	C(9)...C(13)	337.6(46)	16.6(fixed)	1.6	16.6
u_{153}	C(13)...H(20)	345.2(8)	10.4(fixed)	-1.5	10.4
u_{154}	C(12)...H(28)	346.4(16)	10.4(fixed)	-1.4	10.4
u_{155}	C(12)...H(23)	345.1(8)	10.3(fixed)	-1.3	10.3
u_{156}	C(11)...H(21)	278.6(29)	10.4(fixed)	-1.5	10.4
u_{157}	C(11)...H(25)	345.2(8)	10.4(fixed)	-1.3	10.4

u_{158}	C(13)...H(26)	279.5(20)	10.4(fixed)	-1.5	10.4
u_{159}	P(1)...Cl(5)	347.7(10)	12.1(9)	-0.1	11.9
u_{160}	C(9)...H(16)	346.5(8)	10.5(fixed)	-1.8	10.5
u_{161}	C(8)...H(18)	346.6(8)	10.4(fixed)	-1.7	10.4
u_{162}	Si(2)...C(11)	343.5(27)	16.6(Tied to u_{150})	0.3	16.8
u_{163}	P(1)...Cl(6)	350.7(10)	11.8(Tied to u_{159})	-0.2	11.6
u_{164}	C(3)...C(12)	351.6(25)	15.8(fixed)	0.0	15.8
u_{165}	H(10)...H(20)	353.1(53)	32.3(fixed)	-0.3	32.3
u_{166}	C(3)...H(23)	343.5(47)	24.1(fixed)	0.3	24.1
u_{167}	H(10)...H(23)	348.3(59)	30.2(fixed)	-0.5	30.2
u_{168}	Cl(6)...C(11)	354.8(34)	23.2(Tied to u_{170})	1.9	21.1
u_{169}	Si(2)...H(26)	448.1(28)	30.8(fixed)	-0.3	30.8
u_{170}	Cl(7)...C(9)	359.2(41)	30.7(18)	1.7	28.0
u_{171}	H(21)...H(27)	322.2(45)	17.7(fixed)	-1.8	17.7
u_{172}	H(22)...H(28)	430.7(12)	18.3(fixed)	-1.5	18.3
u_{173}	P(1)...Cl(7)	370.9(9)	10.6(Tied to u_{159})	-0.1	10.4
u_{174}	H(22)...H(23)	374.3(23)	17.8(fixed)	-1.4	17.8
u_{175}	H(20)...H(24)	375.2(20)	18.0(fixed)	-1.8	18.0
u_{176}	Si(2)...H(14)	362.3(47)	27.0(fixed)	1.8	27.0
u_{177}	H(18)...H(24)	356.6(66)	25.7(fixed)	4.3	25.7
u_{178}	H(24)...H(26)	258.0(32)	17.7(fixed)	-1.8	17.7
u_{179}	Cl(5)...C(9)	370.9(55)	23.6(Tied to u_{170})	0.7	21.5
u_{180}	H(15)...H(18)	374.3(19)	18.1(fixed)	-1.8	18.1
u_{181}	H(16)...H(19)	377.1(22)	18.5(fixed)	-2.0	18.5
u_{182}	P(1)...H(22)	289.0(23)	10.9(fixed)	-1.7	10.9
u_{183}	H(25)...H(27)	430.1(11)	18.3(fixed)	-1.5	18.3
u_{184}	H(25)...H(28)	371.4(21)	17.8(fixed)	-1.5	17.8
u_{185}	Cl(7)...C(13)	377.2(36)	23.0(Tied to u_{170})	2.3	21.0
u_{186}	H(20)...H(25)	373.2(21)	17.5(fixed)	-1.9	17.5
u_{187}	H(20)...H(28)	377.2(31)	18.0(fixed)	-1.8	18.0
u_{188}	P(1)...H(27)	284.1(20)	11.3(fixed)	-1.6	11.3
u_{189}	H(23)...H(26)	319.5(38)	17.8(fixed)	-1.7	17.8

u_{190}	P(1)...H(15)	375.5(9)	10.9(fixed)	-2.0	10.9
u_{191}	C(3)...Cl(5)	374.9(22)	18.5(Tied to u_{170})	0.4	16.9
u_{192}	C(4)...C(9)	372.3(28)	12.3(fixed)	0.2	12.3
u_{193}	H(16)...H(17)	375.3(21)	18.5(fixed)	-2.3	18.5
u_{194}	H(21)...H(23)	374.1(19)	18.3(fixed)	-1.5	18.3
u_{195}	H(21)...H(26)	254.4(41)	18.4(fixed)	-1.9	18.4
u_{196}	H(16)...H(21)	540.4(51)	40.0(fixed)	3.9	40.0
u_{197}	H(14)...H(18)	378.5(23)	19.0(fixed)	-2.1	19.0
u_{198}	H(10)...H(22)	228.4(46)	27.0(fixed)	0.1	27.0
u_{199}	Cl(5)...C(8)	374.9(46)	29.0(Tied to u_{170})	0.9	26.4
u_{200}	Si(2)...C(13)	384.1(26)	13.3(Tied to u_{150})	0.3	13.5
u_{201}	H(17)...H(23)	397.1(71)	36.5(fixed)	1.5	36.5
u_{202}	P(1)...H(24)	385.3(8)	10.8(fixed)	-1.4	10.8
u_{203}	H(17)...H(25)	333.7(61)	27.7(fixed)	0.5	27.7
u_{204}	P(1)...H(19)	322.4(21)	10.9(fixed)	-1.7	10.9
u_{205}	H(10)...H(24)	389.1(42)	28.3(fixed)	-0.2	28.3
u_{206}	C(3)...H(20)	394.4(41)	26.0(fixed)	-1.2	26.0
u_{207}	C(8)...H(21)	559.5(34)	30.7(fixed)	2.0	30.7
u_{208}	C(4)...Cl(7)	402.3(23)	21.2(Tied to u_{170})	0.4	19.3
u_{209}	Si(2)...C(8)	398.8(30)	16.3(Tied to u_{150})	-0.6	16.5
u_{210}	Cl(7)...C(11)	406.1(64)	37.4(Tied to u_{170})	0.0	34.0
u_{211}	H(19)...H(23)	366.3(81)	33.4(fixed)	0.2	33.4
u_{212}	Si(2)...H(10)	411.4(15)	13.0(fixed)	-1.0	13.0
u_{213}	C(13)...H(19)	408.3(61)	24.8(fixed)	0.2	24.8
u_{214}	H(18)...H(21)	495.6(64)	33.0(fixed)	2.0	33.0
u_{215}	Cl(5)...H(18)	418.5(77)	31.8(fixed)	-1.2	31.8
u_{216}	C(4)...Cl(6)	419.9(25)	18.3(15)	-0.1	16.1
u_{217}	C(13)...H(17)	407.6(49)	23.9(fixed)	-0.4	23.9
u_{218}	C(9)...H(21)	534.0(45)	26.8(fixed)	1.4	26.8
u_{219}	C(3)...Cl(7)	419.8(25)	22.0(Tied to u_{216})	0.1	19.3
u_{220}	Cl(7)...H(25)	426.9(63)	29.0(fixed)	0.8	29.0
u_{221}	H(16)...H(20)	429.8(66)	40.1(fixed)	2.2	40.1

<i>u</i> ₂₂₂	C(4)...C(8)	428.9(13)	11.2(fixed)	-0.9	11.2
<i>u</i> ₂₂₃	C(3)...H(24)	428.1(24)	16.7(fixed)	-1.2	16.7
<i>u</i> ₂₂₄	Si(2)...H(25)	430.5(43)	22.1(fixed)	-0.6	22.1
<i>u</i> ₂₂₅	C(12)...H(16)	436.2(48)	30.0(fixed)	1.1	30.0
<i>u</i> ₂₂₆	H(20)...H(23)	430.2(10)	13.7(fixed)	-2.5	13.7
<i>u</i> ₂₂₇	H(25)...H(26)	377.2(20)	13.7(fixed)	-2.5	13.7
<i>u</i> ₂₂₈	H(21)...H(28)	374.9(26)	13.7(fixed)	-2.6	13.7
<i>u</i> ₂₂₉	H(16)...H(18)	430.7(10)	13.8(fixed)	-2.9	13.8
<i>u</i> ₂₃₀	C(3)...C(11)	430.8(12)	9.5(fixed)	-0.8	9.5
<i>u</i> ₂₃₁	H(10)...C(11)	434.1(21)	17.8(fixed)	-0.7	17.8
<i>u</i> ₂₃₂	C(8)...H(25)	430.5(37)	25.2(fixed)	1.4	25.2
<i>u</i> ₂₃₃	C(4)...H(16)	437.6(26)	20.4(fixed)	-0.2	20.4
<i>u</i> ₂₃₄	C(4)...H(17)	456.9(30)	20.4(fixed)	-1.2	20.4
<i>u</i> ₂₃₅	Cl(5)...H(16)	434.5(69)	36.3(fixed)	-1.4	36.3
<i>u</i> ₂₃₆	C(12)...H(18)	433.1(53)	24.5(fixed)	1.1	24.5
<i>u</i> ₂₃₇	C(3)...H(22)	308.1(37)	18.8(fixed)	-1.9	18.8
<i>u</i> ₂₃₈	H(18)...H(28)	430.7(64)	31.9(fixed)	3.8	31.9
<i>u</i> ₂₃₉	C(9)...H(24)	439.4(49)	19.1(fixed)	-0.3	19.1
<i>u</i> ₂₄₀	Si(2)...H(19)	301.2(36)	16.9(fixed)	-2.0	16.9
<i>u</i> ₂₄₁	Si(2)...H(16)	445.8(44)	25.4(fixed)	-1.8	25.4
<i>u</i> ₂₄₂	H(15)...H(21)	622.4(43)	36.0(fixed)	2.0	36.0
<i>u</i> ₂₄₃	Cl(7)...H(24)	450.9(43)	27.3(fixed)	0.9	27.3
<i>u</i> ₂₄₄	Cl(6)...H(27)	319.8(54)	24.5(fixed)	-0.5	24.5
<i>u</i> ₂₄₅	C(8)...C(12)	457.4(33)	20.8(fixed)	-0.9	20.8
<i>u</i> ₂₄₆	Si(2)...H(27)	352.4(52)	18.3(fixed)	-1.9	18.3
<i>u</i> ₂₄₇	Cl(5)...H(19)	287.6(68)	26.7(fixed)	-1.3	26.7
<i>u</i> ₂₄₈	C(9)...C(12)	455.4(38)	17.3(fixed)	-0.7	17.3
<i>u</i> ₂₄₉	Cl(5)...H(15)	449.1(50)	32.0(fixed)	-1.1	32.0
<i>u</i> ₂₅₀	C(11)...H(18)	446.0(47)	23.4(fixed)	2.3	23.4
<i>u</i> ₂₅₁	C(4)...H(19)	430.7(40)	18.1(fixed)	-1.4	18.1
<i>u</i> ₂₅₂	H(19)...H(21)	614.4(45)	34.4(fixed)	1.7	34.4
<i>u</i> ₂₅₃	C(3)...H(28)	453.3(28)	17.6(fixed)	-0.7	17.6

u_{254}	Cl(7)...H(19)	317.7(65)	32.0(fixed)	-0.9	32.0
u_{255}	Cl(6)...H(23)	463.2(68)	30.0(fixed)	0.7	30.0
u_{256}	C(3)...H(26)	514.4(13)	17.3(fixed)	-1.2	17.3
u_{257}	Si(2)...C(12)	465.1(9)	9.9(fixed)	-0.9	9.9
u_{258}	Cl(7)...H(26)	485.8(71)	41.2(fixed)	-2.4	41.2
u_{259}	C(8)...H(20)	472.7(53)	32.5(fixed)	-1.4	32.5
u_{260}	H(15)...H(25)	469.0(42)	29.8(fixed)	2.1	29.8
u_{261}	H(10)...H(26)	500.3(24)	21.6(fixed)	-1.3	21.6
u_{262}	H(16)...H(25)	471.9(44)	30.5(fixed)	0.5	30.5
u_{263}	Si(2)...H(24)	475.7(27)	17.3(fixed)	-1.3	17.3
u_{264}	C(8)...C(13)	475.3(23)	15.1(fixed)	-0.7	15.1
u_{265}	C(4)...H(14)	475.8(19)	17.8(fixed)	-1.9	17.8
u_{266}	H(10)...H(28)	475.5(29)	21.8(fixed)	-1.4	21.8
u_{267}	Cl(5)...H(10)	481.7(22)	17.9(fixed)	-1.2	17.9
u_{268}	Si(2)...H(20)	483.0(22)	18.7(fixed)	-0.9	18.7
u_{269}	H(14)...H(21)	631.8(31)	31.6(fixed)	-1.3	31.6
u_{270}	Cl(7)...H(27)	458.1(80)	38.3(fixed)	-1.5	38.3
u_{271}	Cl(7)...H(10)	490.7(33)	22.9(fixed)	-0.7	22.9
u_{272}	Si(2)...H(15)	489.9(29)	19.8(fixed)	-2.6	19.8
u_{273}	H(10)...H(27)	472.4(21)	21.8(fixed)	-1.1	21.8
u_{274}	C(9)...H(28)	486.2(51)	24.2(fixed)	0.5	24.2
u_{275}	C(9)...C(11)	492.6(33)	14.5(fixed)	-0.6	14.5
u_{276}	Cl(6)...C(13)	504.3(50)	25.2(13)	-0.9	21.3
u_{277}	H(14)...H(25)	496.8(38)	25.2(fixed)	-0.5	25.2
u_{278}	Si(2)...H(21)	546.9(11)	16.9(fixed)	-1.2	16.9
u_{279}	C(8)...H(23)	493.7(46)	23.7(fixed)	-1.1	23.7
u_{280}	H(18)...H(22)	408.4(68)	29.3(fixed)	0.8	29.3
u_{281}	C(3)...Cl(6)	503.8(11)	11.9(8)	-1.2	10.9
u_{282}	C(4)...H(15)	508.4(16)	15.7(fixed)	-2.2	15.7
u_{283}	C(4)...Cl(5)	505.0(10)	12.0(Tied to u_{281})	-1.0	10.9
u_{284}	H(17)...H(21)	592.0(54)	26.2(fixed)	-1.3	26.2
u_{285}	H(19)...H(24)	512.1(65)	29.0(fixed)	-1.5	29.0

u_{286}	Cl(5)...H(28)	500.1(40)	24.1(fixed)	0.3	24.1
u_{287}	Cl(7)...H(14)	496.9(67)	31.6(fixed)	0.2	31.6
u_{288}	Cl(5)...H(23)	501.8(34)	24.3(fixed)	1.1	24.3
u_{289}	C(13)...H(16)	510.6(29)	21.9(fixed)	-1.3	21.9
u_{290}	Cl(6)...H(17)	647.9(21)	26.5(fixed)	0.7	26.5
u_{291}	C(3)...H(27)	460.9(17)	13.2(fixed)	-2.0	13.2
u_{292}	C(12)...H(19)	530.9(36)	25.3(fixed)	-1.6	25.3
u_{293}	H(18)...H(20)	510.9(48)	26.5(fixed)	-1.5	26.5
u_{294}	C(9)...H(20)	518.1(40)	23.8(fixed)	-2.5	23.8
u_{295}	C(12)...H(15)	526.9(39)	26.9(fixed)	-2.1	26.9
u_{296}	H(17)...H(24)	500.4(56)	25.8(fixed)	-2.7	25.8
u_{297}	H(18)...H(27)	515.4(44)	26.8(fixed)	1.7	26.8
u_{298}	H(17)...H(28)	586.7(51)	34.6(fixed)	0.5	34.6
u_{299}	C(12)...H(14)	526.9(32)	23.6(fixed)	-3.0	23.6
u_{300}	H(18)...H(26)	514.6(55)	25.8(fixed)	-0.2	25.8
u_{301}	Cl(6)...H(20)	528.6(37)	28.6(fixed)	0.1	28.6
u_{302}	Cl(6)...H(14)	520.7(44)	31.2(fixed)	0.3	31.2
u_{303}	Cl(7)...C(8)	523.4(43)	27.0(Tied to u_{276})	-1.4	22.7
u_{304}	C(13)...H(14)	527.2(25)	17.2(fixed)	-1.8	17.2
u_{305}	C(13)...H(15)	532.5(30)	20.9(fixed)	-1.2	20.9
u_{306}	H(14)...H(20)	534.7(54)	35.4(fixed)	-3.1	35.4
u_{307}	C(12)...H(17)	519.0(44)	19.2(fixed)	-2.7	19.2
u_{308}	H(16)...H(22)	382.3(65)	32.6(fixed)	-1.9	32.6
u_{309}	C(9)...H(22)	416.9(51)	21.9(fixed)	-2.0	21.9
u_{310}	Cl(6)...H(18)	533.4(50)	28.1(fixed)	-0.1	28.1
u_{311}	H(14)...H(23)	526.8(52)	27.2(fixed)	-1.0	27.2
u_{312}	Cl(6)...C(12)	540.3(22)	22.4(Tied to u_{276})	-1.1	18.8
u_{313}	C(11)...H(17)	587.4(33)	25.6(fixed)	-1.5	25.6
u_{314}	Cl(6)...C(9)	540.5(22)	17.1(Tied to u_{276})	-1.0	14.4
u_{315}	Cl(5)...H(18)	646.7(22)	29.2(fixed)	-1.7	29.2
u_{316}	H(16)...H(26)	639.1(33)	29.7(fixed)	0.0	29.7
u_{317}	Cl(5)...C(11)	539.8(21)	17.9(Tied to u_{276})	-1.5	15.1

u_{318}	H(15)...H(20)	551.7(60)	37.5(fixed)	-3.5	37.5
u_{319}	Si(2)...H(22)	499.9(19)	13.7(fixed)	-2.1	13.7
u_{320}	C(8)...C(11)	550.0(10)	11.0(fixed)	-2.0	11.0
u_{321}	Cl(7)...C(12)	553.1(20)	21.5(Tied to u_{276})	-1.1	18.1
u_{322}	C(11)...H(16)	553.7(26)	21.5(fixed)	-1.3	21.5
u_{323}	C(9)...H(26)	572.3(38)	19.3(fixed)	-2.0	19.3
u_{324}	H(17)...H(23)	545.8(41)	25.2(fixed)	-2.5	25.2
u_{325}	Cl(5)...C(13)	551.0(21)	18.1(Tied to u_{276})	-0.6	15.2
u_{326}	C(8)...H(22)	404.1(47)	23.3(fixed)	-3.4	23.3
u_{327}	C(8)...H(26)	639.4(13)	20.8(fixed)	-1.7	20.8
u_{328}	H(15)...H(23)	551.6(54)	28.5(fixed)	-1.7	28.5
u_{329}	Cl(6)...C(8)	562.8(29)	23.2(Tied to u_{276})	-1.9	19.6
u_{330}	Cl(6)...H(24)	571.5(57)	26.9(fixed)	-1.9	26.9
u_{331}	Cl(5)...H(25)	568.3(44)	25.5(fixed)	-0.4	25.5
u_{332}	Cl(6)...H(25)	577.7(49)	23.6(fixed)	-2.6	23.6
u_{333}	Cl(6)...H(10)	576.5(15)	14.6(fixed)	-2.2	14.6
u_{334}	C(9)...H(27)	544.0(30)	18.1(fixed)	-1.8	18.1
u_{335}	C(8)...H(24)	577.5(24)	18.6(fixed)	-2.8	18.6
u_{336}	C(8)...H(28)	575.9(27)	18.2(fixed)	-2.1	18.2
u_{337}	C(11)...H(14)	577.1(24)	21.0(fixed)	-2.3	21.0
u_{338}	H(14)...H(26)	675.7(23)	30.1(fixed)	-1.9	30.1
u_{339}	H(19)...H(20)	582.8(37)	30.4(fixed)	-3.9	30.4
u_{340}	H(17)...H(26)	660.1(40)	29.7(fixed)	-2.5	29.7
u_{341}	Cl(6)...H(16)	581.9(50)	32.0(fixed)	-2.3	32.0
u_{342}	H(17)...H(20)	586.0(49)	25.2(fixed)	-3.9	25.2
u_{343}	Cl(7)...H(21)	610.4(27)	21.0(fixed)	-1.4	21.0
u_{344}	H(19)...H(22)	504.4(45)	30.9(fixed)	-2.9	30.9
u_{345}	C(11)...H(19)	529.3(51)	18.1(fixed)	-2.8	18.1
u_{346}	Cl(7)...H(15)	590.7(48)	29.4(fixed)	-2.5	29.4
u_{347}	H(19)...H(28)	505.8(70)	26.1(fixed)	-2.3	26.1
u_{348}	H(14)...H(28)	587.6(42)	27.2(fixed)	-1.5	27.2
u_{349}	H(16)...H(22)	596.1(30)	24.7(fixed)	-2.6	24.7

u_{350}	Cl(7)...H(16)	594.4(42)	24.2(fixed)	-3.4	24.2
u_{351}	Cl(7)...H(20)	602.5(26)	22.6(fixed)	-2.5	22.6
u_{352}	H(16)...H(24)	605.9(35)	26.2(fixed)	-3.1	26.2
u_{353}	Cl(6)...H(22)	605.0(24)	23.0(fixed)	-2.1	23.0
u_{354}	Cl(6)...H(21)	609.0(30)	21.6(fixed)	-2.9	21.6
u_{355}	Cl(7)...H(22)	586.8(26)	23.9(fixed)	-1.5	23.9
u_{356}	H(15)...H(22)	457.1(53)	30.7(fixed)	-4.4	30.7
u_{357}	Cl(5)...C(12)	617.8(11)	12.9(fixed)	-1.7	12.9
u_{358}	H(17)...H(22)	461.6(60)	23.0(fixed)	-4.4	23.0
u_{359}	Cl(5)...H(20)	626.6(26)	22.4(fixed)	-1.7	22.4
u_{360}	H(17)...H(27)	641.6(28)	27.1(fixed)	-3.4	27.1
u_{361}	H(15)...H(24)	631.3(33)	25.1(fixed)	-3.3	25.1
u_{362}	Cl(5)...H(21)	712.5(10)	22.3(fixed)	-1.1	22.3
u_{363}	H(14)...H(22)	489.5(45)	24.3(fixed)	-5.7	24.3
u_{364}	H(16)...H(27)	544.4(39)	24.8(fixed)	-2.8	24.8
u_{365}	C(8)...H(27)	556.8(23)	14.6(fixed)	-3.6	14.6
u_{366}	H(14)...H(24)	633.8(24)	18.8(fixed)	-4.3	18.8
u_{367}	C(11)...H(15)	640.0(12)	14.0(fixed)	-3.9	14.0
u_{368}	H(19)...H(26)	618.7(55)	20.5(fixed)	-4.4	20.5
u_{369}	Cl(6)...H(19)	504.4(36)	16.4(fixed)	-3.9	16.4
u_{370}	Cl(5)...H(27)	535.3(43)	16.7(fixed)	-4.0	16.7
u_{371}	Cl(5)...H(24)	652.7(23)	17.6(fixed)	-2.8	17.6
u_{372}	H(15)...H(26)	723.9(17)	21.8(fixed)	-4.5	21.8
u_{373}	H(19)...H(27)	571.6(50)	23.2(fixed)	-3.8	23.2
u_{374}	H(15)...Cl(6)	664.2(28)	20.9(fixed)	-4.8	20.9
u_{375}	H(15)...H(28)	665.4(29)	19.7(fixed)	-4.2	19.7
u_{376}	H(14)...H(27)	575.6(36)	21.5(fixed)	-4.7	21.5
u_{377}	Cl(5)...H(22)	627.5(25)	14.4(fixed)	-3.7	14.4
u_{378}	H(15)...H(27)	655.2(22)	18.5(fixed)	-5.3	18.5

^a Distances in pm. Values in parentheses are the standard deviations in terms of the last digits.

^b Unrefined amplitudes of vibration were fixed at the values obtained using the B3LYP-D3/Def2TZVP force field.

Table S8. Refined and calculated (B3LYP-D3/Def2TZVP) amplitudes of vibration (u), associated r_a distances and corresponding correction values (k) for the r_{hl} refinement of the Combined Model for +77++&+51-- of **1**.^{a,b}

	Atom pair	r_a	u_{GED}	k	$u_{\text{calc.}}$
u_1	C(9)-H(18)	108.8(3)	7.3(Tied to u_{28})	0.4	7.63
u_2	C(41)-H(53)	108.8(3)	7.3(Tied to u_{28})	0.4	7.63
u_3	C(37)-H(46)	108.8(3)	7.3(Tied to u_{28})	0.4	7.64
u_4	C(13)-H(23)	108.8(3)	7.3(Tied to u_{28})	0.4	7.64
u_5	C(37)-H(45)	108.8(3)	7.3(Tied to u_{28})	0.4	7.65
u_6	C(39)-H(56)	108.8(3)	7.3(Tied to u_{28})	0.4	7.65
u_7	C(40)-H(49)	108.8(3)	7.3(Tied to u_{28})	0.4	7.66
u_8	C(13)-H(25)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_9	C(41)-H(51)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_{10}	C(36)-H(42)	108.8(3)	7.3(Tied to u_{28})	0.4	7.66
u_{11}	C(11)-H(28)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_{12}	C(8)-H(16)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_{13}	C(36)-H(44)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_{14}	C(9)-H(17)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_{15}	C(12)-H(20)	108.8(3)	7.4(Tied to u_{28})	0.4	7.67
u_{16}	C(39)-H(54)	108.8(3)	7.4(Tied to u_{28})	0.4	7.68
u_{17}	C(11)-H(26)	108.8(3)	7.4(Tied to u_{28})	0.4	7.68
u_{18}	C(8)-H(14)	108.8(3)	7.4(Tied to u_{28})	0.4	7.68
u_{19}	C(12)-H(21)	108.8(3)	7.4(Tied to u_{28})	0.4	7.69
u_{20}	C(40)-H(48)	108.8(3)	7.4(Tied to u_{28})	0.4	7.7
u_{21}	C(36)-H(43)	108.8(3)	7.4(Tied to u_{28})	0.4	7.71
u_{22}	C(8)-H(15)	108.8(3)	7.4(Tied to u_{28})	0.4	7.71
u_{23}	C(40)-H(50)	108.8(3)	7.4(Tied to u_{28})	0.4	7.71
u_{24}	C(11)-H(27)	108.8(3)	7.4(Tied to u_{28})	0.4	7.72
u_{25}	C(9)-H(19)	108.8(3)	7.4(Tied to u_{28})	0.4	7.72
u_{26}	C(37)-H(47)	108.8(3)	7.4(Tied to u_{28})	0.4	7.72
u_{27}	C(12)-H(22)	108.8(3)	7.4(Tied to u_{28})	0.4	7.72
u_{28}	C(39)-H(55)	108.8(3)	7.45	0.4	7.72
u_{29}	C(13)-H(24)	108.8(3)	7.4(Tied to u_{28})	0.4	7.73

u_{30}	C(41)-H(52)	108.8(3)	7.4(Tied to u_{28})	0.4	7.73
u_{31}	C(31)-H(38)	108.8(3)	7.4(Tied to u_{28})	0.4	7.75
u_{32}	C(3)-H(10)	108.8(3)	7.4(Tied to u_{28})	0.4	7.75
u_{33}	C(31)-C(37)	153.5(2)	4.0(Tied to u_{37})	0.1	5.25
u_{34}	C(4)-C(13)	153.5(2)	4.0(Tied to u_{37})	0.2	5.27
u_{35}	C(3)-C(9)	153.5(2)	4.0(Tied to u_{37})	0.1	5.27
u_{36}	C(32)-C(41)	153.5(2)	4.0(Tied to u_{37})	0.2	5.29
u_{37}	C(3)-C(8)	153.5(2)	4.03	0.2	5.27
u_{38}	C(31)-C(36)	153.5(2)	4.0(Tied to u_{37})	0.2	5.28
u_{39}	C(4)-C(11)	153.5(2)	4.0(Tied to u_{37})	0.2	5.29
u_{40}	C(32)-C(40)	153.5(2)	4.0(Tied to u_{37})	0.2	5.33
u_{41}	C(32)-C(39)	153.5(2)	4.0(Tied to u_{37})	0.2	5.32
u_{42}	C(4)-C(12)	153.5(2)	4.0(Tied to u_{37})	0.2	5.34
u_{43}	H(17)...H(19)	176.1(7)	12.4(fixed)	0.0	12.41
u_{44}	H(24)...H(25)	176.1(7)	12.4(fixed)	0.0	12.4
u_{45}	H(51)...H(52)	176.1(7)	12.4(fixed)	0.0	12.4
u_{46}	H(49)...H(50)	176.1(7)	12.4(fixed)	0.0	12.37
u_{47}	H(46)...H(47)	176.1(7)	12.4(fixed)	0.0	12.39
u_{48}	H(45)...H(46)	176.1(7)	12.4(fixed)	-0.1	12.38
u_{49}	H(51)...H(53)	176.1(7)	12.4(fixed)	0.0	12.37
u_{50}	H(27)...H(28)	176.1(7)	12.4(fixed)	0.0	12.39
u_{51}	H(21)...H(22)	176.1(7)	12.4(fixed)	0.0	12.41
u_{52}	H(42)...H(43)	176.1(7)	12.4(fixed)	0.0	12.37
u_{53}	H(17)...H(18)	176.1(7)	12.4(fixed)	0.0	12.36
u_{54}	H(48)...H(50)	176.1(7)	12.4(fixed)	0.0	12.42
u_{55}	H(55)...H(56)	176.1(7)	12.4(fixed)	0.0	12.39
u_{56}	H(42)...H(44)	176.1(7)	12.4(fixed)	0.0	12.39
u_{57}	H(45)...H(47)	176.1(7)	12.4(fixed)	-0.1	12.38
u_{58}	H(14)...H(15)	176.1(7)	12.4(fixed)	-0.1	12.4
u_{59}	H(52)...H(53)	176.1(7)	12.4(fixed)	0.0	12.38
u_{60}	H(18)...H(19)	176.1(7)	12.4(fixed)	0.0	12.36
u_{61}	H(23)...H(24)	176.1(7)	12.4(fixed)	0.0	12.38

u_{62}	H(14)...H(16)	176.1(7)	12.4(fixed)	0.0	12.39
u_{63}	H(54)...H(56)	176.1(7)	12.4(fixed)	0.0	12.36
u_{64}	H(26)...H(28)	176.1(7)	12.4(fixed)	0.0	12.4
u_{65}	H(26)...H(27)	176.1(7)	12.4(fixed)	0.0	12.42
u_{66}	H(20)...H(21)	176.1(7)	12.4(fixed)	0.0	12.39
u_{67}	H(23)...H(25)	176.1(7)	12.3(fixed)	0.0	12.33
u_{68}	H(43)...H(44)	176.1(7)	12.4(fixed)	0.0	12.41
u_{69}	H(20)...H(22)	176.1(7)	12.4(fixed)	0.0	12.41
u_{70}	H(54)...H(55)	176.1(7)	12.4(fixed)	0.0	12.42
u_{71}	H(48)...H(49)	176.1(7)	12.4(fixed)	0.0	12.37
u_{72}	H(15)...H(17)	176.1(7)	12.4(fixed)	-0.1	12.41
u_{73}	P(29)-C(31)	187.1(4)	5.3(Tied to u_{74})	0.2	5.91
u_{74}	P(1)-C(3)	187.1(4)	5.35.0	0.2	5.9
u_{75}	P(1)-C(4)	189.0(4)	5.4(Tied to u_{74})	0.2	6.08
u_{76}	P(29)-C(32)	189.7(5)	5.5(Tied to u_{74})	0.2	6.15
u_{77}	Si(2)-Cl(6)	203.7(1)	4.6(Tied to u_{79})	0.2	5.13
u_{78}	Si(30)-Cl(33)	203.7(1)	4.6(Tied to u_{79})	0.2	5.14
u_{79}	Si(30)-Cl(34)	203.7(1)	4.72	0.2	5.17
u_{80}	Si(2)-Cl(5)	203.7(1)	4.7(Tied to u_{79})	0.2	5.18
u_{81}	Si(2)-Cl(7)	203.7(1)	4.7(Tied to u_{79})	0.2	5.25
u_{82}	Si(30)-Cl(35)	203.7(1)	4.7(Tied to u_{79})	0.2	5.26
u_{83}	H(46)...H(53)	188.4(79)	31.1(fixed)	15.5	31.12
u_{84}	C(36)...H(38)	214.5(18)	10.8(Tied to u_{87})	0.0	10.77
u_{85}	C(8)...H(10)	215.1(17)	10.9(Tied to u_{87})	0.0	10.81
u_{86}	C(37)...H(38)	213.7(8)	10.8(Tied to u_{87})	0.0	10.74
u_{87}	C(9)...H(10)	213.7(8)	10.811	0.0	10.78
u_{88}	C(4)...H(24)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.83
u_{89}	C(32)...H(50)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.86
u_{90}	C(31)...H(47)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.85
u_{91}	C(4)...H(27)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.84
u_{92}	C(32)...H(52)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.84
u_{93}	C(3)...H(19)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.85

u_{94}	C(31)...H(43)	217.6(6)	10.9(Tied to u_{87})	-0.1	10.85
u_{95}	C(32)...H(55)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.87
u_{96}	C(4)...H(22)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.9
u_{97}	C(3)...H(15)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.87
u_{98}	C(31)...H(45)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.76
u_{99}	C(3)...H(17)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.79
u_{100}	C(3)...H(14)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.76
u_{101}	C(31)...H(42)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.73
u_{102}	C(32)...H(51)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.76
u_{103}	C(4)...H(25)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.76
u_{104}	C(4)...H(23)	217.6(6)	10.7(Tied to u_{87})	-0.1	10.65
u_{105}	C(3)...H(16)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.77
u_{106}	C(32)...H(54)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.77
u_{107}	C(4)...H(20)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.78
u_{108}	C(31)...H(44)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.8
u_{109}	C(31)...H(46)	217.6(6)	10.9(Tied to u_{87})	-0.2	10.82
u_{110}	C(4)...H(26)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.76
u_{111}	C(4)...H(28)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.76
u_{112}	C(32)...H(48)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.8
u_{113}	C(32)...H(56)	217.6(6)	10.8(Tied to u_{87})	-0.2	10.75
u_{114}	C(32)...H(53)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.74
u_{115}	C(3)...H(18)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.77
u_{116}	C(4)...H(21)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.8
u_{117}	C(32)...H(49)	217.6(6)	10.8(Tied to u_{87})	-0.1	10.8
u_{118}	P(1)-Si(2)	224.6(7)	7.97	0.3	6.01
u_{119}	P(29)-Si(30)	225.0(7)	8.0(Tied to u_{118})	0.3	6.06
u_{120}	H(10)...H(21)	380.0(46)	29.7(fixed)	6.8	29.74
u_{121}	H(46)...H(49)	224.6(119)	40.6(fixed)	9.5	40.58
u_{122}	H(18)...H(25)	222.8(106)	31.2(fixed)	7.0	31.19
u_{123}	P(29)...H(38)	233.0(9)	11.8(fixed)	0.0	11.8
u_{124}	H(38)...H(49)	229.5(61)	30.7(fixed)	4.2	30.73
u_{125}	P(1)...H(10)	234.5(9)	11.9(fixed)	0.0	11.91

u_{126}	H(10)...H(25)	228.8(66)	32.0(fixed)	4.3	31.99
u_{127}	H(38)...H(43)	247.2(25)	18.4(fixed)	0.5	18.36
u_{128}	H(10)...H(19)	305.1(8)	18.2(fixed)	0.4	18.22
u_{129}	H(50)...H(55)	256.9(45)	24.2(fixed)	3.0	24.2
u_{130}	H(18)...H(23)	228.7(90)	33.0(fixed)	8.0	33
u_{131}	H(38)...H(47)	249.0(17)	18.7(fixed)	0.4	18.68
u_{132}	H(20)...H(22)	382.2(33)	24.3(fixed)	3.0	24.27
u_{133}	H(10)...H(16)	247.7(27)	18.5(fixed)	0.3	18.54
u_{134}	H(22)...H(24)	315.2(40)	24.1(fixed)	2.7	24.1
u_{135}	H(50)...H(52)	252.7(35)	24.1(fixed)	2.6	24.07
u_{136}	H(10)...H(15)	251.7(24)	18.7(fixed)	0.2	18.67
u_{137}	C(39)...C(40)	252.7(22)	7.7(Tied to u_{146})	0.0	7.43
u_{138}	C(11)...C(12)	253.5(21)	7.7(Tied to u_{146})	-0.1	7.49
u_{139}	C(39)...C(41)	249.8(9)	7.7(Tied to u_{146})	0.0	7.47
u_{140}	H(38)...H(44)	250.9(27)	19.1(fixed)	0.1	19.07
u_{141}	C(12)...C(13)	249.8(9)	7.7(Tied to u_{146})	0.0	7.44
u_{142}	H(52)...H(55)	258.8(35)	24.7(fixed)	2.9	24.67
u_{143}	H(38)...H(46)	247.2(19)	19.0(fixed)	0.3	18.99
u_{144}	C(11)...C(13)	249.8(9)	7.7(Tied to u_{146})	-0.1	7.49
u_{145}	H(15)...H(19)	304.8(41)	24.7(Tied to u_{146})	3.4	24.71
u_{146}	C(41)...C(40)	249.8(9)	7.9(Tied to u_{146})	-0.1	7.6
u_{147}	H(43)...H(47)	257.2(34)	25.7(fixed)	3.9	25.74
u_{148}	H(24)...H(27)	376.7(20)	24.7(fixed)	2.4	24.71
u_{149}	C(36)...C(37)	252.5(8)	7.9(Tied to u_{146})	-0.1	7.64
u_{150}	C(8)...C(9)	252.5(8)	7.8(Tied to u_{146})	-0.1	7.58
u_{151}	H(10)...H(18)	249.9(19)	18.5(fixed)	0.1	18.49
u_{152}	H(51)...H(56)	250.0(38)	25.4(fixed)	2.8	25.41
u_{153}	H(48)...H(54)	261.5(55)	25.2(fixed)	2.6	25.18
u_{154}	H(23)...H(28)	249.1(38)	24.4(fixed)	2.3	24.38
u_{155}	H(21)...H(25)	302.7(41)	25.0(fixed)	2.5	24.99
u_{156}	H(20)...H(26)	302.4(50)	25.3(fixed)	2.6	25.3
u_{157}	H(38)...H(48)	263.4(66)	33.7(fixed)	3.7	33.72

u_{158}	H(14)...H(17)	320.8(39)	26.8(fixed)	2.8	26.8
u_{159}	H(42)...H(45)	260.3(40)	27.7(fixed)	3.3	27.72
u_{160}	H(49)...H(53)	256.2(39)	25.4(fixed)	2.2	25.41
u_{161}	C(39)...H(50)	275.2(31)	16.2(fixed)	0.3	16.22
u_{162}	C(12)...H(27)	284.9(35)	16.6(fixed)	0.3	16.55
u_{163}	C(40)...H(52)	270.1(21)	16.5(fixed)	0.3	16.5
u_{164}	C(41)...H(55)	273.3(21)	17.2(fixed)	0.3	17.2
u_{165}	C(13)...H(22)	276.3(23)	16.9(fixed)	0.3	16.94
u_{166}	C(11)...H(24)	273.4(21)	16.5(fixed)	0.2	16.48
u_{167}	C(9)...H(15)	274.1(20)	17.3(fixed)	0.4	17.34
u_{168}	C(39)...H(51)	269.4(23)	17.0(fixed)	0.2	17.04
u_{169}	C(40)...H(54)	277.2(36)	17.5(fixed)	0.3	17.52
u_{170}	C(36)...H(47)	275.5(21)	18.0(fixed)	0.3	17.99
u_{171}	C(13)...H(28)	268.6(23)	17.0(fixed)	0.2	16.96
u_{172}	C(40)...H(55)	278.9(31)	17.3(fixed)	0.2	17.32
u_{173}	C(11)...H(20)	277.1(35)	17.3(fixed)	0.2	17.3
u_{174}	C(12)...H(24)	276.6(21)	16.4(fixed)	0.1	16.43
u_{175}	C(12)...H(25)	272.2(23)	16.3(fixed)	0.2	16.34
u_{176}	P(1)...C(12)	272.3(9)	7.47	0.0	8.32
u_{177}	C(11)...H(22)	348.5(17)	17.1(fixed)	0.1	17.08
u_{178}	C(41)...H(49)	271.7(23)	17.0(fixed)	0.1	16.99
u_{179}	H(38)...C(40)	275.7(42)	23.9(fixed)	2.4	23.86
u_{180}	C(8)...H(17)	279.3(21)	17.9(fixed)	0.1	17.93
u_{181}	C(37)...H(43)	278.6(21)	17.7(fixed)	0.2	17.74
u_{182}	C(39)...H(52)	279.5(22)	17.0(fixed)	0.0	17.02
u_{183}	C(41)...H(50)	277.1(22)	16.7(fixed)	0.0	16.71
u_{184}	C(8)...H(19)	276.3(24)	17.1(fixed)	0.1	17.13
u_{185}	C(13)...H(18)	265.0(76)	23.3(fixed)	6.0	23.31
u_{186}	P(29)...C(39)	273.8(9)	7.5(Tied to u_{176})	-0.1	8.43
u_{187}	C(13)...H(27)	345.4(9)	17.2(fixed)	0.0	17.17
u_{188}	C(37)...H(42)	276.9(23)	18.7(fixed)	0.1	18.68
u_{189}	C(39)...H(48)	281.0(36)	16.9(fixed)	0.0	16.92

u_{190}	C(41)...H(56)	275.4(23)	17.6(fixed)	0.1	17.64
u_{191}	C(11)...H(23)	275.3(24)	16.3(fixed)	0.0	16.29
u_{192}	C(13)...H(21)	272.5(21)	17.5(fixed)	0.1	17.51
u_{193}	P(29)...C(40)	276.9(9)	7.5(Tied to u_{176})	0.0	8.45
u_{194}	P(1)...C(8)	277.8(8)	7.5(Tied to u_{176})	-0.2	8.42
u_{195}	C(36)...H(45)	280.1(24)	18.8(fixed)	0.1	18.84
u_{196}	C(12)...H(26)	273.4(31)	17.2(fixed)	0.0	17.19
u_{197}	Cl(35)...H(45)	274.0(59)	28.9(fixed)	15.1	28.86
u_{198}	P(1)...C(11)	277.8(9)	7.6(Tied to u_{176})	0.0	8.61
u_{199}	P(29)...C(36)	279.1(8)	7.4(Tied to u_{176})	-0.1	8.4
u_{200}	Cl(34)...H(56)	264.1(78)	25.3(fixed)	8.4	25.34
u_{201}	C(9)...H(14)	281.5(24)	18.3(fixed)	-0.1	18.26
u_{202}	C(40)...H(53)	278.8(24)	17.2(fixed)	0.0	17.23
u_{203}	Cl(7)...H(23)	282.2(57)	25.5(fixed)	7.2	25.45
u_{204}	C(31)...H(49)	279.5(38)	21.2(fixed)	2.7	21.19
u_{205}	C(4)...H(10)	283.0(25)	18.4(fixed)	0.8	18.35
u_{206}	C(3)...H(25)	279.4(38)	23.3(fixed)	2.7	23.32
u_{207}	Cl(33)...H(42)	277.8(83)	28.9(fixed)	12.7	28.94
u_{208}	P(29)...H(48)	285.4(23)	18.1(fixed)	0.5	18.09
u_{209}	P(29)...H(44)	285.8(21)	18.6(fixed)	0.8	18.62
u_{210}	P(1)...H(26)	375.7(9)	18.5(fixed)	0.5	18.51
u_{211}	P(1)...H(20)	287.2(24)	18.4(fixed)	0.4	18.37
u_{212}	C(37)...H(53)	268.3(58)	28.6(fixed)	6.9	28.59
u_{213}	P(29)...H(54)	286.6(24)	18.6(fixed)	0.5	18.64
u_{214}	P(1)...C(13)	289.5(8)	7.1(Tied to u_{176})	0.0	8
u_{215}	Cl(5)...H(17)	461.0(76)	28.2(fixed)	5.3	28.23
u_{216}	P(1)...H(16)	290.0(22)	18.5(fixed)	0.6	18.48
u_{217}	P(29)...C(41)	291.4(8)	7.2(Tied to u_{176})	0.0	8.15
u_{218}	P(1)...H(21)	372.6(8)	18.7(fixed)	0.3	18.67
u_{219}	C(37)...H(49)	291.2(83)	28.2(fixed)	4.3	28.19
u_{220}	C(9)...H(25)	287.4(72)	24.5(fixed)	3.7	24.46
u_{221}	P(1)...C(9)	292.9(8)	7.1(Tied to u_{176})	-0.1	8

u_{222}	P(29)...C(37)	293.7(8)	7.1(Tied to u_{176})	-0.1	8.04
u_{223}	H(10)...C(12)	295.3(46)	23.6(fixed)	1.8	23.57
u_{224}	C(41)...H(46)	278.9(59)	26.5(fixed)	9.0	26.52
u_{225}	H(20)...H(27)	265.2(54)	27.9(fixed)	-0.5	27.93
u_{226}	H(50)...H(54)	307.5(50)	27.8(fixed)	-0.6	27.78
u_{227}	P(29)...H(56)	293.3(24)	19.3(fixed)	0.2	19.31
u_{228}	H(49)...H(52)	298.1(41)	26.7(fixed)	-0.4	26.72
u_{229}	H(51)...H(55)	299.6(42)	28.4(fixed)	-0.7	28.38
u_{230}	H(24)...H(28)	298.4(41)	26.5(fixed)	-0.5	26.52
u_{231}	Cl(5)...H(14)	298.9(82)	34.3(fixed)	6.2	34.28
u_{232}	Si(30)...H(51)	295.4(36)	23.4(fixed)	3.1	23.38
u_{233}	Cl(6)...H(28)	290.0(83)	29.5(fixed)	4.7	29.47
u_{234}	H(15)...H(17)	256.5(34)	29.8(fixed)	-0.7	29.82
u_{235}	H(19)...H(28)	253.8(38)	26.7(fixed)	-0.6	26.71
u_{236}	C(6)...C(16)	298.6(12)	9.59	0.2	9.41
u_{237}	H(7)...C(17)	294.6(54)	25.2(fixed)	1.1	25.17
u_{238}	H(45)...H(53)	280.0(89)	52.8(fixed)	5.7	52.81
u_{239}	H(38)...H(42)	305.7(14)	12.7(fixed)	-1.7	12.67
u_{240}	Si(1)...H(22)	295.3(45)	24.4(fixed)	3.0	24.4
u_{241}	P(5)...H(14)	302.6(23)	19.9(fixed)	-0.1	19.87
u_{242}	H(7)...H(14)	306.1(14)	12.7(fixed)	-1.7	12.65
u_{243}	H(7)...H(10)	246.3(17)	12.7(fixed)	-1.6	12.7
u_{244}	H(38)...H(45)	305.2(8)	12.7(fixed)	-1.8	12.67
u_{245}	H(42)...H(47)	308.0(40)	31.7(fixed)	-1.0	31.66
u_{246}	C(31)...C(32)	303.3(11)	9.1(Tied to u_{236})	0.2	9.01
u_{247}	C(40)...H(46)	304.1(91)	33.9(fixed)	5.9	33.87
u_{248}	P(29)...H(49)	302.9(24)	16.8(fixed)	0.1	16.77
u_{249}	Cl(35)...H(51)	294.5(90)	35.8(fixed)	4.2	35.81
u_{250}	Cl(34)...H(51)	317.4(94)	37.2(fixed)	4.5	37.17
u_{251}	Si(1)...H(10)	445.1(23)	26.6(fixed)	2.5	26.63
u_{252}	C(6)...H(27)	445.3(32)	24.5(fixed)	2.7	24.54
u_{253}	P(5)...H(22)	307.7(24)	17.3(fixed)	0.1	17.33

u_{254}	C(32)...H(38)	310.8(32)	19.1(fixed)	0.5	19.07
u_{255}	C(32)...H(46)	304.2(40)	24.6(fixed)	5.8	24.56
u_{256}	H(20)...H(27)	254.4(35)	26.6(fixed)	-1.0	26.61
u_{257}	H(48)...H(55)	318.9(49)	27.1(fixed)	-1.0	27.14
u_{258}	H(43)...H(45)	317.7(40)	30.8(fixed)	-1.4	30.82
u_{259}	Cl(4)...H(9)	302.1(75)	36.7(fixed)	4.5	36.72
u_{260}	P(29)...H(42)	311.0(23)	18.7(fixed)	-0.2	18.69
u_{261}	P(5)...H(9)	309.2(21)	16.9(fixed)	0.6	16.87
u_{262}	P(29)...H(53)	308.8(21)	17.4(fixed)	0.4	17.44
u_{263}	P(5)...H(19)	310.4(22)	17.0(fixed)	0.2	16.95
u_{264}	P(5)...H(18)	310.4(22)	16.7(fixed)	0.2	16.65
u_{265}	H(52)...H(56)	318.2(39)	27.7(fixed)	-1.1	27.71
u_{266}	P(29)...H(46)	312.8(21)	18.2(fixed)	0.6	18.16
u_{267}	H(23)...H(28)	375.7(28)	27.0(fixed)	-1.1	27.02
u_{268}	H(18)...H(24)	372.1(25)	25.6(fixed)	-1.1	25.61
u_{269}	H(11)...H(14)	261.4(40)	28.7(fixed)	-1.4	28.7
u_{270}	C(31)...C(40)	319.7(27)	12.7(fixed)	0.6	12.69
u_{271}	H(50)...H(53)	319.6(40)	25.9(fixed)	-1.1	25.93
u_{272}	P(29)...H(51)	316.6(22)	16.6(fixed)	0.2	16.61
u_{273}	Cl(35)...H(53)	322.6(86)	40.5(fixed)	4.3	40.53
u_{274}	P(29)...H(45)	321.1(21)	18.2(fixed)	0.2	18.18
u_{275}	P(5)...H(10)	386.8(8)	17.6(fixed)	-0.1	17.58
u_{276}	C(31)...H(48)	329.6(54)	25.9(fixed)	0.4	25.9
u_{277}	Si(1)...C(6)	325.9(7)	9.910	0.1	9.86
u_{278}	Si(30)...H(45)	323.0(44)	26.3(fixed)	5.4	26.31
u_{279}	Cl(2)...H(23)	436.7(54)	37.3(fixed)	3.0	37.25
u_{280}	C(6)...C(17)	322.9(28)	14.3(fixed)	0.6	14.29
u_{281}	Si(30)...C(31)	327.6(7)	9.2(Tied to u_{277})	0.1	9.12
u_{282}	Cl(33)...Cl(35)	324.5(24)	10.34	-0.1	10.15
u_{283}	Cl(34)...Cl(35)	327.1(11)	10.3(Tied to u_{282})	-0.1	10.14
u_{284}	Cl(2)...Cl(4)	327.8(11)	10.3(Tied to u_{282})	-0.1	10.11
u_{285}	Cl(2)...Cl(3)	327.8(11)	10.2(Tied to u_{282})	-0.2	10.01

u_{286}	Cl(33)...Cl(34)	327.8(11)	10.3(Tied to u_{282})	-0.2	10.12
u_{287}	Si(30)...C(32)	329.6(7)	9.7(Tied to u_{277})	0.1	9.64
u_{288}	Cl(3)...Cl(4)	326.5(24)	10.5(Tied to u_{282})	-0.1	10.26
u_{289}	Cl(4)...H(10)	446.1(58)	40.6(fixed)	2.8	40.6
u_{290}	Cl(4)...H(22)	325.7(116)	43.4(fixed)	3.8	43.37
u_{291}	C(8)...H(18)	319.6(80)	29.1(fixed)	2.4	29.14
u_{292}	Si(1)...C(16)	331.3(7)	9.5(Tied to u_{277})	0.1	9.49
u_{293}	Si(30)...H(42)	325.1(55)	28.8(fixed)	4.3	28.77
u_{294}	Si(1)...H(18)	334.6(48)	21.8(fixed)	2.4	21.83
u_{295}	H(11)...H(19)	379.8(86)	32.1(fixed)	3.7	32.14
u_{296}	C(31)...H(53)	326.8(44)	22.1(fixed)	2.4	22.07
u_{297}	Si(1)...H(9)	336.6(60)	27.4(fixed)	1.0	27.44
u_{298}	Si(1)...C(8)	337.9(24)	14.715	0.6	14.51
u_{299}	Si(30)...C(41)	342.4(25)	16.216	0.6	16.08
u_{300}	H(9)...C(16)	336.7(50)	20.7(fixed)	2.8	20.71
u_{301}	C(40)...H(56)	348.0(17)	10.4(fixed)	-1.6	10.39
u_{302}	H(47)...H(49)	344.8(78)	33.8(fixed)	3.8	33.78
u_{303}	C(41)...H(54)	345.8(8)	10.4(fixed)	-1.6	10.44
u_{304}	C(39)...H(49)	347.9(17)	10.4(fixed)	-1.3	10.38
u_{305}	C(8)...C(17)	338.8(55)	16.6(fixed)	1.6	16.56
u_{306}	C(17)...H(26)	345.8(8)	10.4(fixed)	-1.5	10.41
u_{307}	H(22)...C(25)	348.2(16)	10.4(fixed)	-1.4	10.44
u_{308}	H(18)...C(25)	345.7(8)	10.3(fixed)	-1.3	10.33
u_{309}	C(21)...H(27)	280.9(30)	10.4(fixed)	-1.5	10.42
u_{310}	H(19)...C(21)	345.8(8)	10.4(fixed)	-1.3	10.4
u_{311}	C(17)...H(23)	280.5(22)	10.4(fixed)	-1.5	10.4
u_{312}	C(40)...H(51)	345.6(8)	10.5(fixed)	-1.4	10.5
u_{313}	C(39)...H(53)	345.5(9)	10.4(fixed)	-1.4	10.38
u_{314}	C(41)...H(48)	345.7(8)	10.4(fixed)	-1.4	10.43
u_{315}	Cl(3)...P(5)	345.6(10)	12.19	-0.1	11.94
u_{316}	C(8)...H(13)	347.6(8)	10.5(fixed)	-1.8	10.48
u_{317}	C(37)...H(44)	347.8(8)	10.5(fixed)	-1.9	10.49

u_{318}	C(36)...H(46)	347.7(8)	10.6(fixed)	-2.0	10.58
u_{319}	H(9)...C(12)	347.8(8)	10.4(fixed)	-1.7	10.44
u_{320}	P(29)...Cl(33)	347.3(10)	11.8(Tied to u_{315})	-0.1	11.64
u_{321}	Si(30)...H(56)	332.0(58)	22.2(fixed)	2.7	22.21
u_{322}	Si(1)...C(21)	341.8(35)	17.0(Tied to u_{298})	0.3	16.79
u_{323}	Cl(2)...P(5)	348.6(10)	11.7(Tied to u_{315})	-0.2	11.57
u_{324}	P(29)...Cl(34)	349.0(10)	11.8(Tied to u_{315})	-0.1	11.62
u_{325}	C(6)...C(25)	350.7(33)	15.8(fixed)	0.0	15.84
u_{326}	H(7)...H(26)	352.9(66)	32.3(fixed)	-0.3	32.29
u_{327}	C(6)...H(18)	343.2(57)	24.1(fixed)	0.3	24.1
u_{328}	Si(30)...H(53)	353.1(58)	30.8(fixed)	0.4	30.79
u_{329}	C(32)...C(37)	349.6(30)	16.2(fixed)	1.0	16.15
u_{330}	H(7)...H(18)	345.1(77)	30.2(fixed)	-0.5	30.21
u_{331}	Cl(2)...C(21)	344.7(47)	21.1(Tied to u_{339})	1.9	21.12
u_{332}	Cl(35)...C(41)	353.3(67)	28.4(Tied to u_{334})	2.3	28.05
u_{333}	H(46)...H(52)	344.2(58)	32.2(fixed)	8.7	32.24
u_{334}	Cl(33)...C(36)	355.0(68)	23.423	4.2	23.13
u_{335}	Si(1)...H(23)	446.9(34)	30.8(fixed)	-0.3	30.82
u_{336}	Cl(35)...C(37)	361.1(52)	22.2(Tied to u_{334})	5.0	21.9
u_{337}	C(37)...C(40)	363.2(65)	21.8(fixed)	0.9	21.76
u_{338}	C(37)...C(41)	349.3(47)	22.3(fixed)	2.5	22.29
u_{339}	Cl(4)...C(8)	352.0(52)	27.929	1.7	27.97
u_{340}	Cl(33)...H(44)	357.1(98)	52.3(fixed)	3.1	52.32
u_{341}	H(46)...H(51)	348.8(88)	32.7(fixed)	5.6	32.65
u_{342}	H(50)...H(56)	376.4(28)	17.5(fixed)	-1.9	17.54
u_{343}	H(24)...H(27)	325.8(47)	17.7(fixed)	-1.8	17.68
u_{344}	H(49)...H(55)	377.1(28)	18.3(fixed)	-1.4	18.31
u_{345}	Si(30)...C(37)	369.1(34)	18.6(Tied to u_{299})	0.6	18.49
u_{346}	H(22)...H(28)	432.2(13)	18.3(fixed)	-1.5	18.34
u_{347}	H(48)...H(52)	372.9(20)	17.6(fixed)	-1.6	17.55
u_{348}	Cl(4)...P(5)	369.4(9)	10.5(Tied to u_{315})	-0.1	10.4
u_{349}	Cl(34)...C(39)	359.5(65)	20.4(Tied to u_{334})	2.2	20.18

u_{350}	H(18)...H(28)	375.1(24)	17.8(fixed)	-1.4	17.81
u_{351}	H(50)...H(51)	374.4(23)	18.3(fixed)	-1.7	18.29
u_{352}	H(20)...H(26)	375.5(22)	18.0(fixed)	-1.8	18.02
u_{353}	Si(1)...H(14)	368.1(59)	27.0(fixed)	1.8	26.95
u_{354}	H(9)...H(20)	359.7(82)	25.7(fixed)	4.3	25.7
u_{355}	H(53)...H(55)	376.3(20)	18.0(fixed)	-1.7	17.97
u_{356}	Si(30)...C(36)	367.6(40)	21.3(Tied to u_{299})	0.1	21.16
u_{357}	P(29)...Cl(35)	370.7(9)	10.6(Tied to u_{315})	-0.1	10.5
u_{358}	H(20)...H(23)	260.0(35)	17.7(fixed)	-1.8	17.67
u_{359}	Cl(3)...C(8)	376.2(74)	24.6(Tied to u_{372})	0.7	21.52
u_{360}	H(52)...H(54)	378.2(22)	18.3(fixed)	-1.9	18.34
u_{361}	H(9)...H(15)	375.9(20)	18.1(fixed)	-1.8	18.11
u_{362}	H(44)...H(47)	376.6(21)	18.6(fixed)	-2.1	18.55
u_{363}	H(11)...H(13)	378.5(23)	18.5(fixed)	-2.0	18.46
u_{364}	P(5)...H(28)	289.5(24)	10.9(fixed)	-1.7	10.87
u_{365}	H(43)...H(46)	377.2(22)	18.9(fixed)	-2.3	18.87
u_{366}	H(19)...H(24)	431.1(12)	18.3(fixed)	-1.5	18.33
u_{367}	H(51)...H(54)	371.7(23)	18.0(fixed)	-2.0	17.98
u_{368}	H(46)...H(48)	373.4(104)	37.3(fixed)	2.1	37.26
u_{369}	P(29)...H(55)	373.9(8)	11.0(fixed)	-1.9	10.96
u_{370}	H(49)...H(54)	378.9(34)	18.1(fixed)	-1.6	18.12
u_{371}	H(19)...H(22)	371.0(23)	17.8(fixed)	-1.5	17.82
u_{372}	Cl(4)...C(17)	377.1(47)	24.019	2.3	20.97
u_{373}	P(29)...H(50)	375.7(9)	11.2(fixed)	-1.4	11.18
u_{374}	C(31)...C(41)	367.2(30)	13.6(fixed)	0.2	13.55
u_{375}	H(19)...H(26)	374.1(23)	17.5(fixed)	-1.9	17.53
u_{376}	P(29)...H(43)	375.9(9)	11.3(fixed)	-2.0	11.33
u_{377}	H(22)...H(26)	380.0(32)	18.0(fixed)	-1.8	18
u_{378}	H(53)...H(56)	372.7(25)	18.5(fixed)	-1.6	18.51
u_{379}	P(5)...H(24)	284.1(22)	11.3(fixed)	-1.6	11.29
u_{380}	H(18)...H(23)	319.4(39)	17.8(fixed)	-1.7	17.82
u_{381}	P(5)...H(15)	376.1(8)	10.9(fixed)	-2.0	10.92

u_{382}	Cl(3)...C(6)	378.6(34)	19.3(Tied to u_{372})	0.4	16.88
u_{383}	H(48)...H(56)	379.8(34)	18.3(fixed)	-2.0	18.26
u_{384}	Cl(35)...H(46)	378.5(91)	51.1(fixed)	3.0	51.05
u_{385}	C(8)...C(16)	373.5(34)	12.3(fixed)	0.2	12.28
u_{386}	H(10)...H(13)	376.8(22)	18.5(fixed)	-2.3	18.54
u_{387}	H(18)...H(27)	374.5(21)	18.3(fixed)	-1.5	18.26
u_{388}	H(49)...H(51)	374.8(23)	17.9(fixed)	-1.8	17.86
u_{389}	H(23)...H(27)	256.8(45)	18.4(fixed)	-1.9	18.35
u_{390}	H(42)...H(46)	378.3(23)	19.2(fixed)	-2.5	19.16
u_{391}	H(44)...H(45)	379.1(25)	19.3(fixed)	-2.3	19.34
u_{392}	H(38)...H(53)	364.1(72)	27.4(fixed)	1.0	27.43
u_{393}	H(38)...H(50)	379.2(44)	25.7(fixed)	0.5	25.67
u_{394}	H(13)...H(27)	535.4(68)	40.0(fixed)	3.9	40.03
u_{395}	H(9)...H(14)	379.8(24)	19.0(fixed)	-2.1	19.01
u_{396}	H(7)...H(28)	226.9(61)	27.0(fixed)	0.1	26.95
u_{397}	H(48)...H(53)	376.6(25)	18.2(fixed)	-1.6	18.23
u_{398}	H(47)...H(53)	359.1(65)	28.2(fixed)	3.4	28.18
u_{399}	Cl(3)...C(12)	382.0(61)	30.2(Tied to u_{372})	0.9	26.42
u_{400}	C(41)...H(45)	363.3(76)	45.8(fixed)	1.4	45.83
u_{401}	H(46)...H(50)	375.4(95)	38.5(fixed)	5.8	38.5
u_{402}	H(45)...H(49)	378.9(98)	35.3(fixed)	0.3	35.33
u_{403}	Si(1)...C(17)	383.3(34)	13.6(Tied to u_{298})	0.3	13.48
u_{404}	H(10)...H(18)	397.5(87)	36.5(fixed)	1.5	36.53
u_{405}	P(5)...H(20)	385.5(8)	10.8(fixed)	-1.4	10.78
u_{406}	H(10)...H(19)	332.8(67)	27.7(fixed)	0.5	27.73
u_{407}	P(5)...H(11)	322.7(21)	10.9(fixed)	-1.7	10.9
u_{408}	P(29)...H(52)	386.9(8)	10.9(fixed)	-1.5	10.89
u_{409}	P(29)...H(47)	387.6(8)	11.0(fixed)	-1.9	10.98
u_{410}	C(32)...Cl(34)	389.1(40)	19.717	0.7	17.67
u_{411}	H(7)...H(20)	384.1(51)	28.3(fixed)	-0.2	28.25
u_{412}	Cl(34)...C(41)	398.1(76)	32.9(Tied to u_{410})	0.6	29.48
u_{413}	Si(30)...C(39)	380.6(38)	13.5(Tied to u_{299})	-0.1	13.45

u_{414}	C(6)...H(26)	394.3(49)	26.0(fixed)	-1.2	25.96
u_{415}	Si(30)...H(44)	392.3(67)	39.4(fixed)	-1.6	39.4
u_{416}	C(32)...H(45)	389.6(54)	32.2(fixed)	-0.7	32.17
u_{417}	C(12)...H(27)	556.4(44)	30.7(fixed)	2.0	30.71
u_{418}	Si(30)...H(46)	400.5(62)	38.6(fixed)	-1.1	38.6
u_{419}	Cl(4)...C(16)	403.0(30)	22.1(Tied to u_{372})	0.4	19.33
u_{420}	Cl(35)...H(42)	394.0(112)	60.7(fixed)	2.6	60.7
u_{421}	H(38)...C(41)	396.8(53)	21.3(fixed)	-0.5	21.26
u_{422}	C(31)...Cl(33)	400.3(43)	20.9(Tied to u_{410})	0.0	18.7
u_{423}	Si(1)...C(12)	402.1(37)	16.6(Tied to u_{298})	-0.6	16.45
u_{424}	C(31)...Cl(35)	403.6(32)	22.2(Tied to u_{410})	0.7	19.89
u_{425}	C(37)...H(48)	409.9(81)	28.4(fixed)	-1.0	28.43
u_{426}	Cl(33)...H(45)	406.6(108)	54.8(fixed)	2.1	54.84
u_{427}	Cl(4)...C(21)	408.0(89)	34.8(Tied to u_{555})	0.0	34.01
u_{428}	H(11)...H(18)	371.1(96)	33.4(fixed)	0.2	33.44
u_{429}	Si(1)...H(7)	409.9(17)	13.0(fixed)	-1.0	12.97
u_{430}	H(45)...H(51)	387.1(89)	50.9(fixed)	2.2	50.93
u_{431}	H(11)...C(17)	411.7(73)	24.8(fixed)	0.2	24.81
u_{432}	H(9)...H(27)	499.6(81)	33.0(fixed)	2.0	33.03
u_{433}	Cl(3)...H(9)	421.5(99)	31.8(fixed)	-1.2	31.81
u_{434}	Cl(2)...C(16)	413.0(34)	18.4(Tied to u_{372})	-0.1	16.06
u_{435}	H(10)...C(17)	407.5(56)	23.9(fixed)	-0.4	23.87
u_{436}	C(37)...H(51)	401.3(71)	28.7(fixed)	1.2	28.74
u_{437}	C(8)...H(27)	535.8(55)	26.8(fixed)	1.4	26.83
u_{438}	Si(30)...H(38)	418.7(9)	12.1(fixed)	-1.8	12.05
u_{439}	Cl(4)...C(6)	415.2(32)	22.1(Tied to u_{372})	0.1	19.34
u_{440}	C(32)...Cl(35)	418.9(42)	22.0(Tied to u_{410})	0.3	19.72
u_{441}	Cl(4)...H(19)	424.3(84)	29.0(fixed)	0.8	29.04
u_{442}	Cl(34)...H(54)	406.0(89)	32.2(fixed)	-0.1	32.16
u_{443}	H(13)...H(26)	425.4(83)	40.1(fixed)	2.2	40.08
u_{444}	C(31)...H(50)	425.5(26)	14.7(fixed)	-1.3	14.65
u_{445}	C(31)...H(51)	417.2(47)	21.5(fixed)	-0.8	21.45

<i>u</i> ₄₄₆	C(12)...C(16)	427.6(16)	11.2(fixed)	-0.9	11.23
<i>u</i> ₄₄₇	H(38)...H(54)	436.0(49)	26.0(fixed)	1.4	25.97
<i>u</i> ₄₄₈	C(40)...H(47)	433.0(64)	27.8(fixed)	-0.5	27.76
<i>u</i> ₄₄₉	C(6)...H(20)	426.4(27)	16.7(fixed)	-1.2	16.74
<i>u</i> ₄₅₀	Si(1)...H(19)	428.9(54)	22.1(fixed)	-0.6	22.11
<i>u</i> ₄₅₁	C(36)...H(49)	427.4(40)	23.1(fixed)	0.7	23.12
<i>u</i> ₄₅₂	H(13)...C(25)	431.3(64)	30.0(fixed)	1.1	29.95
<i>u</i> ₄₅₃	H(18)...H(26)	431.3(12)	13.7(fixed)	-2.5	13.65
<i>u</i> ₄₅₄	H(19)...H(23)	378.9(22)	13.7(fixed)	-2.5	13.69
<i>u</i> ₄₅₅	H(48)...H(51)	431.2(12)	13.8(fixed)	-2.5	13.75
<i>u</i> ₄₅₆	H(53)...H(54)	431.1(12)	13.7(fixed)	-2.6	13.66
<i>u</i> ₄₅₇	H(49)...H(56)	432.2(13)	13.6(fixed)	-2.6	13.64
<i>u</i> ₄₅₈	H(22)...H(27)	376.8(28)	13.7(fixed)	-2.6	13.69
<i>u</i> ₄₅₉	H(38)...C(39)	436.3(32)	19.7(fixed)	-0.1	19.74
<i>u</i> ₄₆₀	C(31)...C(39)	432.1(12)	9.9(fixed)	-0.7	9.91
<i>u</i> ₄₆₁	H(44)...H(46)	432.1(12)	13.9(fixed)	-3.2	13.86
<i>u</i> ₄₆₂	H(9)...H(13)	432.1(12)	13.8(fixed)	-2.9	13.8
<i>u</i> ₄₆₃	C(6)...C(21)	430.1(14)	9.5(fixed)	-0.8	9.46
<i>u</i> ₄₆₄	H(7)...C(21)	432.1(23)	17.8(fixed)	-0.7	17.82
<i>u</i> ₄₆₅	C(12)...H(19)	427.2(43)	25.2(fixed)	1.4	25.16
<i>u</i> ₄₆₆	H(13)...C(16)	435.0(34)	20.4(fixed)	-0.2	20.44
<i>u</i> ₄₆₇	Si(30)...H(54)	425.3(56)	24.7(fixed)	-1.4	24.66
<i>u</i> ₄₆₈	H(10)...C(16)	457.4(33)	20.4(fixed)	-1.2	20.37
<i>u</i> ₄₆₉	C(40)...H(45)	438.1(78)	31.0(fixed)	-2.5	30.99
<i>u</i> ₄₇₀	Cl(3)...H(13)	439.7(85)	36.3(fixed)	-1.4	36.28
<i>u</i> ₄₇₁	C(32)...C(36)	439.4(10)	9.5(fixed)	-1.6	9.45
<i>u</i> ₄₇₂	H(9)...C(25)	436.8(69)	24.5(fixed)	1.1	24.46
<i>u</i> ₄₇₃	Cl(34)...H(53)	454.0(90)	37.9(fixed)	-1.6	37.85
<i>u</i> ₄₇₄	C(31)...H(54)	446.6(29)	18.9(fixed)	-0.3	18.89
<i>u</i> ₄₇₅	C(6)...H(28)	307.2(47)	18.8(fixed)	-1.9	18.76
<i>u</i> ₄₇₆	Cl(34)...H(55)	435.4(74)	27.0(fixed)	0.2	27
<i>u</i> ₄₇₇	C(37)...H(52)	431.5(51)	28.0(fixed)	0.9	27.95

<i>u</i> ₄₇₈	C(36)...H(48)	453.2(55)	31.7(fixed)	-1.0	31.73
<i>u</i> ₄₇₉	H(9)...H(22)	428.9(83)	31.9(fixed)	3.8	31.9
<i>u</i> ₄₈₀	C(8)...H(20)	440.8(59)	19.1(fixed)	-0.3	19.11
<i>u</i> ₄₈₁	H(44)...H(48)	452.1(69)	42.2(fixed)	0.0	42.15
<i>u</i> ₄₈₂	Si(30)...H(52)	447.1(24)	17.6(fixed)	-1.6	17.57
<i>u</i> ₄₈₃	C(32)...H(47)	445.9(28)	18.2(fixed)	-1.5	18.17
<i>u</i> ₄₈₄	Si(1)...H(11)	301.1(36)	16.9(fixed)	-2.0	16.88
<i>u</i> ₄₈₅	Si(1)...H(13)	449.1(51)	25.4(fixed)	-1.8	25.4
<i>u</i> ₄₈₆	H(15)...H(27)	618.4(54)	36.0(fixed)	2.0	35.98
<i>u</i> ₄₈₇	Cl(4)...H(20)	452.8(51)	27.3(fixed)	0.9	27.31
<i>u</i> ₄₈₈	Cl(2)...H(24)	309.3(73)	24.5(fixed)	-0.5	24.52
<i>u</i> ₄₈₉	Cl(35)...H(47)	449.1(57)	24.0(fixed)	0.6	24.03
<i>u</i> ₄₉₀	C(12)...C(25)	454.3(43)	20.8(fixed)	-0.9	20.82
<i>u</i> ₄₉₁	Si(1)...H(24)	349.7(68)	18.3(fixed)	-1.9	18.3
<i>u</i> ₄₉₂	Cl(35)...H(52)	445.7(75)	32.1(fixed)	0.0	32.13
<i>u</i> ₄₉₃	C(37)...H(50)	451.4(68)	26.1(fixed)	-0.5	26.09
<i>u</i> ₄₉₄	Cl(33)...H(43)	448.2(77)	24.4(fixed)	-0.1	24.4
<i>u</i> ₄₉₅	Cl(3)...H(11)	294.2(90)	26.7(fixed)	-1.3	26.74
<i>u</i> ₄₉₆	C(8)...C(25)	457.0(49)	17.3(fixed)	-0.7	17.34
<i>u</i> ₄₉₇	Cl(3)...H(15)	458.8(65)	32.0(fixed)	-1.1	31.99
<i>u</i> ₄₉₈	H(9)...C(21)	446.2(59)	23.4(fixed)	2.3	23.43
<i>u</i> ₄₉₉	H(11)...C(16)	433.1(47)	18.1(fixed)	-1.4	18.11
<i>u</i> ₅₀₀	Cl(35)...C(36)	454.8(79)	39.045	-1.5	43.66
<i>u</i> ₅₀₁	H(11)...H(27)	617.2(53)	34.4(fixed)	1.7	34.39
<i>u</i> ₅₀₂	C(6)...H(22)	452.5(35)	17.6(fixed)	-0.7	17.61
<i>u</i> ₅₀₃	C(36)...C(40)	463.5(26)	15.8(fixed)	-1.4	15.82
<i>u</i> ₅₀₄	C(41)...H(47)	447.1(50)	22.3(fixed)	-0.9	22.3
<i>u</i> ₅₀₅	Cl(4)...H(11)	313.2(84)	32.0(fixed)	-0.9	31.96
<i>u</i> ₅₀₆	C(32)...H(44)	460.4(21)	18.7(fixed)	-2.1	18.67
<i>u</i> ₅₀₇	H(47)...H(48)	470.2(87)	36.7(fixed)	-1.7	36.7
<i>u</i> ₅₀₈	Si(30)...C(40)	462.5(12)	10.3(fixed)	-0.8	10.32
<i>u</i> ₅₀₉	Cl(2)...H(18)	455.6(99)	30.0(fixed)	0.7	30

u_{510}	C(31)...H(52)	457.9(29)	17.3(fixed)	-1.4	17.3
u_{511}	Cl(33)...C(37)	461.6(81)	34.7(Tied to u_{500})	-2.1	38.84
u_{512}	H(43)...H(49)	464.9(46)	27.6(fixed)	1.9	27.56
u_{513}	C(39)...H(46)	457.0(38)	24.3(fixed)	4.1	24.34
u_{514}	C(6)...H(23)	514.0(14)	17.3(fixed)	-1.2	17.3
u_{515}	Si(1)...C(25)	464.7(10)	9.9(fixed)	-0.9	9.85
u_{516}	Cl(4)...H(23)	489.0(93)	41.2(fixed)	-2.4	41.24
u_{517}	C(12)...H(26)	470.2(65)	32.5(fixed)	-1.4	32.45
u_{518}	Cl(34)...H(52)	477.0(82)	33.5(fixed)	-0.9	33.53
u_{519}	Si(30)...H(47)	468.5(30)	18.3(fixed)	-2.5	18.31
u_{520}	H(15)...H(19)	464.9(51)	29.8(fixed)	2.1	29.81
u_{521}	H(44)...H(49)	468.0(55)	30.9(fixed)	-1.1	30.89
u_{522}	H(45)...H(52)	453.8(84)	49.7(fixed)	-1.2	49.73
u_{523}	Si(30)...H(43)	469.5(36)	20.3(fixed)	-2.7	20.27
u_{524}	H(7)...H(23)	498.4(27)	21.6(fixed)	-1.3	21.62
u_{525}	C(31)...H(56)	468.4(21)	17.6(fixed)	-1.2	17.58
u_{526}	H(38)...H(51)	467.0(54)	23.3(fixed)	-2.2	23.34
u_{527}	H(13)...H(19)	467.7(60)	30.5(fixed)	0.5	30.49
u_{528}	H(38)...H(52)	470.6(56)	26.4(fixed)	-1.3	26.4
u_{529}	Si(1)...H(20)	475.8(31)	17.3(fixed)	-1.3	17.27
u_{530}	C(12)...C(17)	473.7(29)	15.1(fixed)	-0.7	15.13
u_{531}	Cl(35)...H(56)	456.1(94)	30.8(fixed)	1.0	30.77
u_{532}	H(14)...C(16)	476.4(19)	17.8(fixed)	-1.9	17.75
u_{533}	H(7)...H(22)	472.9(37)	21.8(fixed)	-1.4	21.77
u_{534}	C(36)...H(53)	466.1(45)	25.8(fixed)	0.3	25.8
u_{535}	Si(30)...H(49)	480.3(31)	18.9(fixed)	-0.5	18.86
u_{536}	Si(30)...H(55)	473.6(37)	17.8(fixed)	-2.1	17.78
u_{537}	C(32)...H(42)	477.6(25)	17.2(fixed)	-2.3	17.15
u_{538}	C(40)...H(44)	484.5(42)	27.1(fixed)	-1.9	27.11
u_{539}	Cl(3)...H(7)	485.1(32)	17.9(fixed)	-1.2	17.9
u_{540}	Si(1)...H(26)	483.4(28)	18.7(fixed)	-0.9	18.69
u_{541}	H(14)...H(27)	630.6(37)	31.6(fixed)	-1.3	31.63

u_{542}	Cl(4)...H(24)	459.2(111)	38.3(fixed)	-1.5	38.25
u_{543}	H(45)...H(48)	492.1(79)	30.2(fixed)	-4.6	30.23
u_{544}	Cl(4)...H(7)	484.6(40)	22.9(fixed)	-0.7	22.87
u_{545}	Si(1)...H(15)	493.3(34)	19.8(fixed)	-2.6	19.82
u_{546}	H(38)...H(56)	494.8(28)	23.0(fixed)	-1.8	23.02
u_{547}	H(43)...H(48)	505.5(66)	36.1(fixed)	-0.9	36.09
u_{548}	H(42)...H(53)	479.4(66)	37.1(fixed)	0.9	37.07
u_{549}	H(7)...H(24)	471.9(23)	21.8(fixed)	-1.1	21.83
u_{550}	Cl(33)...H(38)	496.1(37)	18.6(fixed)	-2.5	18.6
u_{551}	C(8)...H(22)	485.5(66)	24.2(fixed)	0.5	24.17
u_{552}	Si(30)...H(48)	498.1(18)	16.9(fixed)	-1.3	16.9
u_{553}	C(8)...C(21)	492.8(42)	14.5(fixed)	-0.6	14.51
u_{554}	H(42)...H(49)	495.7(42)	23.7(fixed)	-1.0	23.72
u_{555}	Cl(2)...C(17)	496.7(71)	21.822	-0.9	21.27
u_{556}	H(14)...H(19)	495.6(40)	25.2(fixed)	-0.5	25.17
u_{557}	C(37)...C(39)	497.5(25)	14.8(fixed)	-0.2	14.78
u_{558}	Si(1)...H(27)	546.7(11)	16.9(fixed)	-1.2	16.9
u_{559}	C(12)...H(18)	494.6(55)	23.7(fixed)	-1.1	23.73
u_{560}	Cl(35)...H(38)	502.2(30)	18.9(fixed)	-2.2	18.94
u_{561}	H(9)...H(28)	412.9(89)	29.3(fixed)	0.8	29.29
u_{562}	H(38)...H(55)	510.7(38)	23.5(fixed)	-1.1	23.49
u_{563}	Cl(2)...C(6)	502.8(9)	11.9(Tied to u_{607})	-1.2	10.85
u_{564}	Cl(33)...H(51)	498.6(37)	23.8(fixed)	0.5	23.79
u_{565}	H(15)...C(16)	506.9(19)	15.7(fixed)	-2.2	15.66
u_{566}	C(31)...Cl(34)	504.0(9)	11.6(Tied to u_{579})	-1.3	10.66
u_{567}	Cl(3)...C(16)	504.3(10)	12.0(Tied to u_{607})	-1.0	10.93
u_{568}	H(10)...H(27)	593.0(64)	26.2(fixed)	-1.3	26.24
u_{569}	H(11)...H(20)	516.0(78)	29.0(fixed)	-1.5	28.99
u_{570}	C(32)...Cl(33)	505.6(9)	12.0(Tied to u_{579})	-1.5	11.05
u_{571}	Cl(3)...H(22)	498.3(43)	24.1(fixed)	0.3	24.08
u_{572}	Cl(4)...H(14)	498.3(87)	31.6(fixed)	0.2	31.56
u_{573}	Cl(3)...H(18)	506.6(43)	24.3(fixed)	1.1	24.27

<i>u</i> ₅₇₄	H(13)...C(17)	507.8(41)	21.9(fixed)	-1.3	21.88
<i>u</i> ₅₇₅	H(46)...H(55)	506.7(48)	29.2(fixed)	5.0	29.15
<i>u</i> ₅₇₆	Cl(2)...H(10)	646.0(20)	26.5(fixed)	0.7	26.49
<i>u</i> ₅₇₇	C(40)...H(43)	518.7(34)	21.1(fixed)	-1.2	21.14
<i>u</i> ₅₇₈	H(46)...H(56)	499.6(45)	26.2(fixed)	2.9	26.17
<i>u</i> ₅₇₉	Cl(35)...C(39)	499.6(67)	25.021	-0.9	22.99
<i>u</i> ₅₈₀	C(6)...H(24)	460.6(19)	13.2(fixed)	-2.0	13.2
<i>u</i> ₅₈₁	C(31)...H(55)	516.3(15)	13.3(fixed)	-2.0	13.33
<i>u</i> ₅₈₂	C(36)...C(41)	506.9(29)	15.7(fixed)	-1.8	15.7
<i>u</i> ₅₈₃	Cl(33)...H(56)	503.3(62)	27.7(fixed)	0.7	27.67
<i>u</i> ₅₈₄	H(46)...H(54)	511.9(47)	27.3(fixed)	2.0	27.26
<i>u</i> ₅₈₅	H(47)...H(50)	517.0(70)	32.0(fixed)	-2.0	31.95
<i>u</i> ₅₈₆	H(11)...C(25)	533.0(44)	25.3(fixed)	-1.6	25.34
<i>u</i> ₅₈₇	C(32)...H(43)	519.0(14)	13.7(fixed)	-2.5	13.65
<i>u</i> ₅₈₈	H(9)...H(26)	514.4(60)	26.5(fixed)	-1.5	26.47
<i>u</i> ₅₈₉	Cl(34)...H(45)	513.1(44)	24.3(fixed)	1.6	24.25
<i>u</i> ₅₉₀	C(8)...H(26)	519.9(49)	23.8(fixed)	-2.5	23.8
<i>u</i> ₅₉₁	H(15)...C(25)	523.3(50)	26.9(fixed)	-2.1	26.91
<i>u</i> ₅₉₂	H(44)...H(54)	525.3(49)	34.5(fixed)	0.2	34.5
<i>u</i> ₅₉₃	H(47)...H(51)	505.2(75)	29.2(fixed)	-3.0	29.17
<i>u</i> ₅₉₄	H(10)...H(20)	500.1(63)	25.8(fixed)	-2.7	25.84
<i>u</i> ₅₉₅	H(9)...H(24)	515.1(55)	26.8(fixed)	1.7	26.78
<i>u</i> ₅₉₆	Cl(35)...H(44)	518.6(89)	52.5(fixed)	-5.7	52.54
<i>u</i> ₅₉₇	H(10)...H(22)	585.6(67)	34.6(fixed)	0.5	34.59
<i>u</i> ₅₉₈	H(14)...C(25)	525.4(40)	23.6(fixed)	-3.0	23.56
<i>u</i> ₅₉₉	Cl(35)...H(49)	528.9(62)	30.1(fixed)	1.1	30.13
<i>u</i> ₆₀₀	H(45)...H(50)	523.3(87)	37.7(fixed)	-4.2	37.73
<i>u</i> ₆₀₁	C(40)...H(42)	529.1(24)	16.6(fixed)	-3.2	16.6
<i>u</i> ₆₀₂	H(9)...H(23)	516.3(67)	25.8(fixed)	-0.2	25.84
<i>u</i> ₆₀₃	H(42)...H(48)	532.3(48)	30.3(fixed)	-3.8	30.25
<i>u</i> ₆₀₄	Cl(34)...H(42)	519.6(52)	24.6(fixed)	-0.3	24.58
<i>u</i> ₆₀₅	Cl(2)...H(26)	525.1(52)	28.6(fixed)	0.1	28.59

u_{606}	Cl(2)...H(14)	530.1(57)	31.2(fixed)	0.3	31.16
u_{607}	Cl(4)...C(12)	522.0(56)	24.922	-1.4	22.71
u_{608}	H(14)...C(17)	528.1(28)	17.2(fixed)	-1.8	17.19
u_{609}	Cl(33)...H(46)	530.5(86)	48.1(fixed)	-6.2	48.07
u_{610}	H(15)...C(17)	530.3(38)	20.9(fixed)	-1.2	20.87
u_{611}	H(14)...H(26)	533.4(64)	35.4(fixed)	-3.1	35.37
u_{612}	H(47)...H(52)	519.4(56)	29.5(fixed)	-2.2	29.45
u_{613}	H(10)...C(25)	519.9(55)	19.2(fixed)	-2.7	19.2
u_{614}	C(41)...H(42)	523.6(50)	26.9(fixed)	-1.5	26.94
u_{615}	H(13)...H(28)	376.1(81)	32.6(fixed)	-1.9	32.6
u_{616}	C(8)...H(28)	418.7(68)	21.9(fixed)	-2.0	21.87
u_{617}	Cl(2)...H(9)	526.5(55)	28.1(fixed)	-0.1	28.08
u_{618}	Cl(35)...H(43)	532.1(82)	44.2(fixed)	-3.1	44.24
u_{619}	Cl(33)...H(47)	534.9(86)	39.9(fixed)	-3.8	39.87
u_{620}	H(14)...H(18)	530.4(60)	27.2(fixed)	-1.0	27.22
u_{621}	C(39)...H(45)	527.9(48)	30.6(fixed)	-1.8	30.56
u_{622}	Cl(35)...C(40)	540.0(45)	23.9(Tied to u_{630})	-0.3	22.05
u_{623}	Cl(2)...C(25)	535.0(29)	20.118	-1.1	18.84
u_{624}	Cl(34)...C(40)	540.4(36)	18.4(Tied to u_{630})	-0.7	16.96
u_{625}	C(37)...H(54)	539.7(31)	19.0(fixed)	-1.2	19.04
u_{626}	H(43)...H(53)	526.3(52)	27.8(fixed)	0.3	27.81
u_{627}	Cl(33)...H(53)	535.2(62)	31.4(fixed)	-1.3	31.42
u_{628}	C(37)...H(56)	530.1(33)	18.5(fixed)	-0.6	18.53
u_{629}	H(10)...C(21)	587.3(40)	25.6(fixed)	-1.5	25.58
u_{630}	Cl(33)...C(41)	539.3(25)	17.113	-1.5	15.79
u_{631}	Si(30)...H(50)	544.6(12)	14.0(fixed)	-2.0	14.04
u_{632}	Cl(2)...C(8)	537.8(21)	15.4(Tied to u_{623})	-1.0	14.43
u_{633}	Cl(3)...H(23)	644.1(26)	29.2(fixed)	-1.7	29.18
u_{634}	H(13)...H(23)	637.4(41)	29.7(fixed)	0.0	29.65
u_{635}	H(44)...H(53)	531.2(40)	26.1(fixed)	-2.7	26.12
u_{636}	Cl(3)...C(21)	536.5(26)	16.1(Tied to u_{623})	-1.5	15.07
u_{637}	C(36)...H(54)	548.4(34)	24.4(fixed)	-1.7	24.43

u_{638}	C(39)...H(44)	546.6(29)	23.8(fixed)	-2.2	23.83
u_{639}	H(15)...H(26)	548.8(73)	37.5(fixed)	-3.5	37.48
u_{640}	Si(1)...H(28)	499.5(20)	13.7(fixed)	-2.1	13.68
u_{641}	C(36)...C(39)	549.3(13)	12.6(fixed)	-2.5	12.56
u_{642}	C(12)...C(21)	549.9(11)	11.0(fixed)	-2.0	10.95
u_{643}	C(36)...H(51)	539.4(50)	25.8(fixed)	-2.3	25.79
u_{644}	Cl(4)...C(25)	553.7(25)	19.4(Tied to u_{623})	-1.1	18.14
u_{645}	H(13)...C(21)	552.8(31)	21.5(fixed)	-1.3	21.54
u_{646}	C(8)...H(23)	573.5(46)	19.3(fixed)	-2.0	19.29
u_{647}	H(42)...H(51)	536.1(71)	36.5(fixed)	-0.9	36.53
u_{648}	H(13)...H(18)	545.6(50)	25.2(fixed)	-2.5	25.24
u_{649}	Cl(3)...C(17)	553.7(30)	16.3(Tied to u_{623})	-0.6	15.23
u_{650}	Cl(34)...C(37)	552.9(34)	16.7(Tied to u_{630})	-1.1	15.41
u_{651}	C(12)...H(28)	399.7(58)	23.3(fixed)	-3.4	23.32
u_{652}	H(45)...H(56)	539.2(59)	33.9(fixed)	-0.6	33.88
u_{653}	Cl(33)...C(39)	551.8(43)	19.5(Tied to u_{630})	-1.8	17.97
u_{654}	C(12)...H(23)	639.0(15)	20.8(fixed)	-1.7	20.77
u_{655}	H(15)...H(18)	552.1(67)	28.5(fixed)	-1.7	28.45
u_{656}	C(41)...H(44)	553.4(24)	18.9(fixed)	-3.7	18.93
u_{657}	Cl(34)...C(36)	554.5(36)	17.7(Tied to u_{630})	-2.4	16.3
u_{658}	Cl(34)...H(46)	559.8(65)	35.2(fixed)	-0.4	35.22
u_{659}	Cl(34)...H(44)	556.5(66)	33.9(fixed)	-2.7	33.91
u_{660}	C(37)...H(55)	564.8(33)	20.4(fixed)	-0.8	20.4
u_{661}	Cl(2)...C(12)	568.1(37)	20.9(Tied to u_{623})	-1.9	19.55
u_{662}	C(36)...H(50)	571.5(26)	17.4(fixed)	-3.8	17.39
u_{663}	Cl(2)...H(20)	563.8(76)	26.9(fixed)	-1.9	26.88
u_{664}	H(44)...H(56)	567.2(40)	30.8(fixed)	-2.4	30.77
u_{665}	Cl(3)...H(19)	571.2(53)	25.5(fixed)	-0.4	25.45
u_{666}	C(36)...H(56)	570.7(26)	21.3(fixed)	-2.7	21.28
u_{667}	Cl(2)...H(19)	570.9(69)	23.6(fixed)	-2.6	23.61
u_{668}	Cl(2)...H(7)	573.5(16)	14.6(fixed)	-2.2	14.62
u_{669}	C(8)...H(24)	543.8(38)	18.1(fixed)	-1.8	18.13

<i>u</i> ₆₇₀	C(12)...H(20)	575.4(29)	18.6(fixed)	-2.8	18.57
<i>u</i> ₆₇₁	Cl(33)...H(54)	568.5(68)	31.5(fixed)	-2.1	31.46
<i>u</i> ₆₇₂	Cl(34)...H(38)	576.8(14)	14.7(fixed)	-2.1	14.71
<i>u</i> ₆₇₃	Cl(34)...H(48)	574.6(35)	20.5(fixed)	-1.3	20.48
<i>u</i> ₆₇₄	Cl(35)...H(55)	567.9(77)	30.1(fixed)	-1.9	30.13
<i>u</i> ₆₇₅	C(12)...H(22)	576.9(29)	18.2(fixed)	-2.1	18.17
<i>u</i> ₆₇₆	H(14)...C(21)	579.0(25)	21.0(fixed)	-2.3	20.96
<i>u</i> ₆₇₇	H(14)...H(23)	677.4(24)	30.1(fixed)	-1.9	30.05
<i>u</i> ₆₇₈	H(11)...H(26)	584.8(41)	30.4(fixed)	-3.9	30.39
<i>u</i> ₆₇₉	H(10)...H(23)	660.8(46)	29.7(fixed)	-2.5	29.71
<i>u</i> ₆₈₀	Cl(2)...H(13)	587.8(57)	32.0(fixed)	-2.3	31.99
<i>u</i> ₆₈₁	Cl(35)...H(54)	572.9(64)	25.4(fixed)	-3.3	25.38
<i>u</i> ₆₈₂	H(10)...H(26)	587.5(60)	25.2(fixed)	-3.9	25.17
<i>u</i> ₆₈₃	C(41)...H(43)	580.4(34)	18.5(fixed)	-2.6	18.51
<i>u</i> ₆₈₄	H(45)...H(54)	580.1(42)	28.2(fixed)	-3.5	28.17
<i>u</i> ₆₈₅	Cl(4)...H(27)	611.9(34)	21.0(fixed)	-1.4	20.99
<i>u</i> ₆₈₆	C(39)...H(42)	582.8(25)	19.7(fixed)	-3.5	19.65
<i>u</i> ₆₈₇	H(44)...H(50)	592.9(44)	29.3(fixed)	-4.7	29.33
<i>u</i> ₆₈₈	H(11)...H(28)	506.3(59)	30.9(fixed)	-2.9	30.91
<i>u</i> ₆₈₉	Cl(34)...H(49)	591.1(40)	21.3(fixed)	-1.8	21.31
<i>u</i> ₆₉₀	H(44)...H(51)	583.0(45)	28.5(fixed)	-4.1	28.51
<i>u</i> ₆₉₁	H(11)...C(21)	530.9(61)	18.1(fixed)	-2.8	18.12
<i>u</i> ₆₉₂	Cl(34)...H(50)	597.3(46)	22.3(fixed)	-1.1	22.3
<i>u</i> ₆₉₃	H(42)...H(54)	593.0(38)	29.5(fixed)	-3.8	29.46
<i>u</i> ₆₉₄	C(39)...H(47)	595.7(25)	17.6(fixed)	-2.9	17.63
<i>u</i> ₆₉₅	H(42)...H(56)	585.1(44)	27.9(fixed)	-2.4	27.85
<i>u</i> ₆₉₆	Cl(4)...H(15)	588.6(61)	29.4(fixed)	-2.5	29.44
<i>u</i> ₆₉₇	H(11)...H(22)	507.2(86)	26.1(fixed)	-2.3	26.12
<i>u</i> ₆₉₈	H(14)...H(22)	591.2(47)	27.2(fixed)	-1.5	27.21
<i>u</i> ₆₉₉	H(13)...H(22)	596.7(31)	24.7(fixed)	-2.6	24.71
<i>u</i> ₇₀₀	Cl(4)...H(13)	593.5(51)	24.2(fixed)	-3.4	24.18
<i>u</i> ₇₀₁	Cl(4)...H(26)	604.2(34)	22.6(fixed)	-2.5	22.61

<i>u</i> ₇₀₂	H(13)...H(20)	602.3(47)	26.2(fixed)	-3.1	26.21
<i>u</i> ₇₀₃	Cl(35)...H(48)	605.7(38)	22.6(fixed)	-2.1	22.57
<i>u</i> ₇₀₄	Cl(2)...H(28)	600.9(27)	23.0(fixed)	-2.1	23.04
<i>u</i> ₇₀₅	Cl(2)...H(27)	602.8(38)	21.6(fixed)	-2.9	21.64
<i>u</i> ₇₀₆	Cl(4)...H(28)	586.1(34)	23.9(fixed)	-1.5	23.94
<i>u</i> ₇₀₇	Cl(35)...H(50)	608.3(55)	27.6(fixed)	-1.2	27.57
<i>u</i> ₇₀₈	H(45)...H(55)	598.8(60)	36.8(fixed)	-3.0	36.77
<i>u</i> ₇₀₉	C(36)...H(52)	604.0(28)	17.5(fixed)	-4.0	17.51
<i>u</i> ₇₁₀	H(15)...H(28)	452.0(66)	30.7(fixed)	-4.4	30.66
<i>u</i> ₇₁₁	H(43)...H(50)	623.3(36)	23.3(fixed)	-3.6	23.26
<i>u</i> ₇₁₂	Cl(3)...C(25)	616.6(12)	12.9(fixed)	-1.7	12.88
<i>u</i> ₇₁₃	H(10)...H(28)	462.7(78)	23.0(fixed)	-4.4	23.02
<i>u</i> ₇₁₄	Cl(33)...C(40)	619.4(14)	12.5(fixed)	-2.4	12.48
<i>u</i> ₇₁₅	H(47)...H(54)	631.1(37)	23.3(fixed)	-3.3	23.32
<i>u</i> ₇₁₆	Cl(3)...H(26)	623.9(29)	22.4(fixed)	-1.7	22.38
<i>u</i> ₇₁₇	H(10)...H(24)	641.6(34)	27.1(fixed)	-3.4	27.08
<i>u</i> ₇₁₈	H(43)...H(54)	636.4(41)	26.6(fixed)	-3.1	26.58
<i>u</i> ₇₁₉	H(15)...H(20)	628.2(39)	25.1(fixed)	-3.3	25.11
<i>u</i> ₇₂₀	Cl(3)...H(27)	711.9(11)	22.3(fixed)	-1.1	22.33
<i>u</i> ₇₂₁	H(14)...H(28)	486.6(54)	24.3(fixed)	-5.7	24.28
<i>u</i> ₇₂₂	Cl(33)...H(49)	627.5(39)	21.6(fixed)	-2.0	21.57
<i>u</i> ₇₂₃	Cl(33)...H(48)	631.0(26)	22.1(fixed)	-2.2	22.05
<i>u</i> ₇₂₄	H(43)...H(51)	622.9(54)	26.9(fixed)	-4.0	26.87
<i>u</i> ₇₂₅	H(13)...H(24)	544.2(46)	24.8(fixed)	-2.8	24.76
<i>u</i> ₇₂₆	C(39)...H(43)	638.6(18)	15.8(fixed)	-3.9	15.82
<i>u</i> ₇₂₇	H(42)...H(50)	635.4(25)	18.2(fixed)	-5.8	18.15
<i>u</i> ₇₂₈	C(12)...H(24)	557.0(25)	14.6(fixed)	-3.6	14.6
<i>u</i> ₇₂₉	H(14)...H(20)	634.5(26)	18.8(fixed)	-4.3	18.83
<i>u</i> ₇₃₀	H(42)...H(52)	627.4(49)	27.4(fixed)	-4.4	27.39
<i>u</i> ₇₃₁	H(15)...C(21)	639.5(13)	14.0(fixed)	-3.9	14.01
<i>u</i> ₇₃₂	C(36)...H(55)	644.1(14)	14.6(fixed)	-4.7	14.61
<i>u</i> ₇₃₃	H(47)...H(56)	635.0(30)	19.7(fixed)	-4.0	19.69

<i>u</i> ₇₃₄	H(44)...H(55)	646.5(31)	25.5(fixed)	-5.0	25.51
<i>u</i> ₇₃₅	H(11)...H(23)	621.5(65)	20.5(fixed)	-4.4	20.46
<i>u</i> ₇₃₆	Cl(33)...H(52)	646.3(23)	17.1(fixed)	-4.2	17.13
<i>u</i> ₇₃₇	Cl(2)...H(11)	504.3(36)	16.4(fixed)	-3.9	16.39
<i>u</i> ₇₃₈	Cl(3)...H(24)	528.5(54)	16.7(fixed)	-4.0	16.69
<i>u</i> ₇₃₉	H(44)...H(52)	649.5(24)	20.2(fixed)	-5.9	20.19
<i>u</i> ₇₄₀	Cl(3)...H(20)	655.8(29)	17.6(fixed)	-2.8	17.57
<i>u</i> ₇₄₁	H(15)...H(23)	723.1(20)	21.8(fixed)	-4.5	21.8
<i>u</i> ₇₄₂	H(47)...H(55)	659.5(34)	23.0(fixed)	-3.5	23.01
<i>u</i> ₇₄₃	Cl(34)...H(47)	658.1(30)	16.4(fixed)	-4.7	16.44
<i>u</i> ₇₄₄	Cl(33)...H(55)	654.1(41)	19.8(fixed)	-4.5	19.81
<i>u</i> ₇₄₅	H(11)...H(24)	572.1(59)	23.2(fixed)	-3.8	23.18
<i>u</i> ₇₄₆	Cl(34)...H(43)	660.8(33)	16.9(fixed)	-5.4	16.94
<i>u</i> ₇₄₇	Cl(2)...H(15)	669.6(35)	20.9(fixed)	-4.8	20.92
<i>u</i> ₇₄₈	H(15)...H(22)	666.0(35)	19.7(fixed)	-4.2	19.72
<i>u</i> ₇₄₉	H(43)...H(56)	668.9(25)	22.0(fixed)	-4.9	22.02
<i>u</i> ₇₅₀	H(43)...H(52)	671.1(35)	21.9(fixed)	-4.4	21.88
<i>u</i> ₇₅₁	H(14)...H(24)	577.1(38)	21.5(fixed)	-4.7	21.52
<i>u</i> ₇₅₂	H(42)...H(55)	680.6(26)	20.1(fixed)	-5.9	20.14
<i>u</i> ₇₅₃	Cl(3)...H(28)	627.3(28)	14.4(fixed)	-3.7	14.36
<i>u</i> ₇₅₄	Cl(33)...H(50)	714.1(11)	14.3(fixed)	-4.3	14.34
<i>u</i> ₇₅₅	H(15)...H(24)	655.4(25)	18.5(fixed)	-5.3	18.45
<i>u</i> ₇₅₆	H(43)...H(55)	727.7(22)	18.5(fixed)	-5.7	18.5

^a Distances in pm. Values in parentheses are the standard deviations in terms of the last digits.

^b Unrefined amplitudes of vibration were fixed at the values obtained using the B3LYP-D3/Def2TZVP force field.

Table S9. Least squares correlation matrix (x 100) for the GED refinement of conformer +77+.^a

	<i>p</i> ₁₈	<i>u</i> ₃₉	<i>u</i> ₁₄₃	<i>k</i> ₂
<i>p</i> ₆			-54	
<i>p</i> ₁₇	-52			
<i>u</i> ₃₇		54		
<i>u</i> ₃₉				54

^a Only elements with absolute values $\geq 50\%$ are shown; *k*₂ is a scale factor.**Table S10.** Least squares correlation matrix (x 100) for the GED refinement of conformer +51--.^a

	<i>p</i> ₃	<i>p</i> ₁₄	<i>p</i> ₁₈	<i>u</i> ₁₆₃	<i>k</i> ₂
<i>p</i> ₁	52	-51			
<i>p</i> ₂		-59			
<i>p</i> ₁₇			-74		
<i>u</i> ₄₀					55
<i>u</i> ₁₄₇				50	

^a Only elements with absolute values $\geq 50\%$ are shown; *k*₂ is a scale factor.**Table S11.** Least squares correlation matrix (x 100) for the GED refinement of conformer -91(-).^a

	<i>p</i> ₁₈	<i>u</i> ₄₂	<i>k</i> ₂
<i>p</i> ₁₇	-68		
<i>u</i> ₃₇		53	
<i>u</i> ₄₂		100	55

^a Only elements with absolute values $\geq 50\%$ are shown; *k*₂ is a scale factor.

Table S12. Least squares correlation matrix (x 100) for the GED refinement of conformer +143-
-.^a

	<i>p</i> ₂₅	<i>k</i> ₂
<i>p</i> ₂₃	56	
<i>u</i> ₄₀		56

^a Only elements with absolute values $\geq 50\%$ are shown; *k*₂ is a scale factor.

Table S13. Least squares correlation matrix (x 100) for the GED refinement of conformer +165+-.^a

	<i>k</i> ₂
<i>u</i> ₄₁	52

^a Only elements with absolute values $\geq 50\%$ are shown; *k*₂ is a scale factor.

Table S14. Least squares correlation matrix (x 100) for the GED refinement of the combined model with the two conformers +77++&+51--.^a

	<i>p</i> ₁₄	<i>p</i> ₁₈	<i>u</i> ₈₁	<i>u</i> ₈₄	<i>u</i> ₃₁₁
<i>p</i> ₁				52	
<i>p</i> ₂	-50				
<i>p</i> ₁₇		-63			
<i>u</i> ₇₃			52		
<i>u</i> ₂₈₄					54

^a Only elements with absolute values $\geq 50\%$ are shown.

Table S15. Experimental coordinates from the GED refinement of conformer +77++.^a

Atom	x	y	z
P(1)	0.0	0.0	0.0
Si(2)	225.5	0.0	0.0
C(3)	-45.7	0.0	181.8
C(4)	-52.7	-169.6	-65.1
Cl(5)	288.5	156.2	115.0
Cl(6)	293.3	33.5	-189.5
Cl(7)	-325.5	162.6	72.0
C(8)	-69.2	144.6	226.4
C(9)	-47.1	72.0	280.1
H(10)	-140.4	-53.1	180.4
C(11)	-22.3	195.4	-196.2
C(12)	-203.0	-156.2	-91.1
C(13)	-28.3	-286.6	30.6
H(14)	23.0	201.7	222.6
H(15)	-106.7	147.9	328.3
H(16)	-141.8	193.5	162.3
H(17)	-2.4	76.9	378.9
H(18)	-67.1	173.5	247.1
H(19)	-142.1	20.1	288.7
H(20)	-223.0	-76.6	-162.1
H(21)	-243.5	-248.4	-131.7
H(22)	-256.2	-133.6	0.8
H(23)	-77.0	294.9	55.5
H(24)	-59.9	-380.4	-14.1
H(25)	-83.7	-273.1	123.0
H(26)	-19.9	-280.6	-248.7
H(27)	-16.3	109.1	-261.8
H(28)	-127.2	216.0	-177.3

^a Coordinates are in pm.

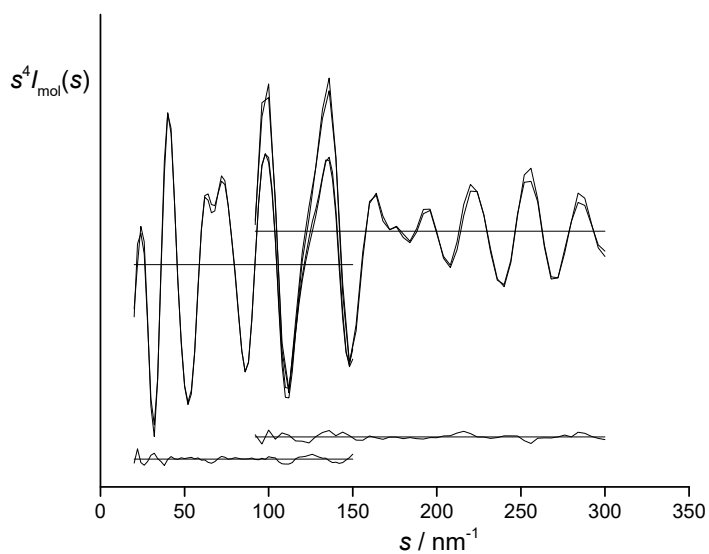


Figure S1: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for the conformer +77++.

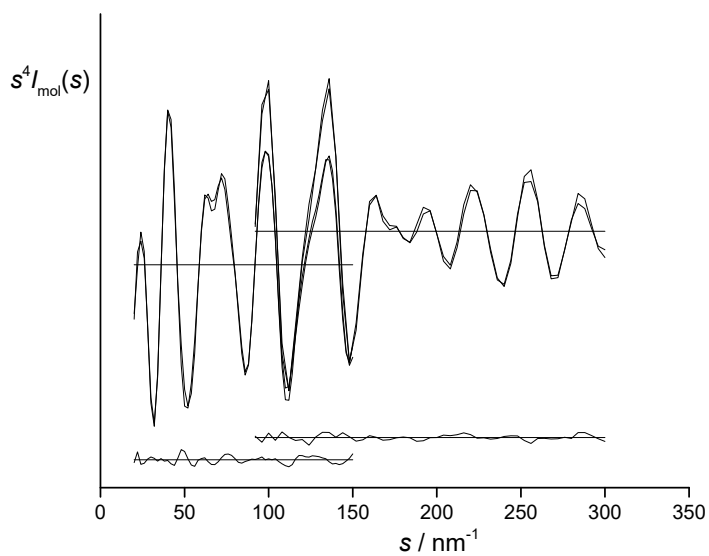


Figure S2: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for the conformer -91(-).

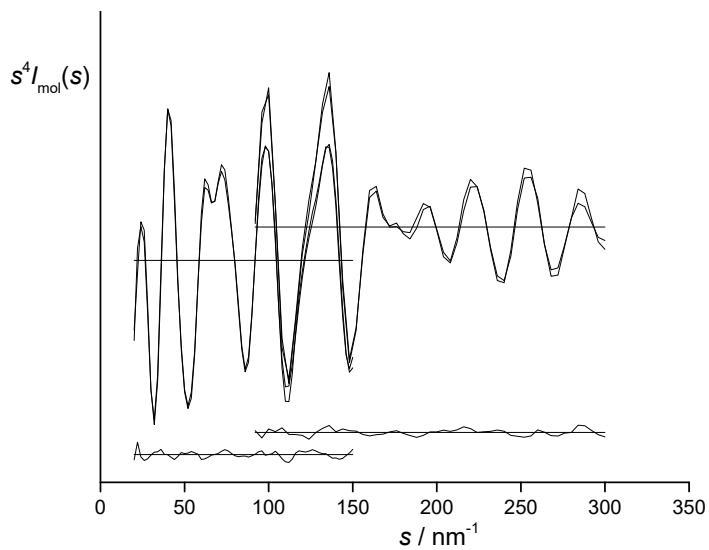


Figure S3: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for the conformer +165+-.

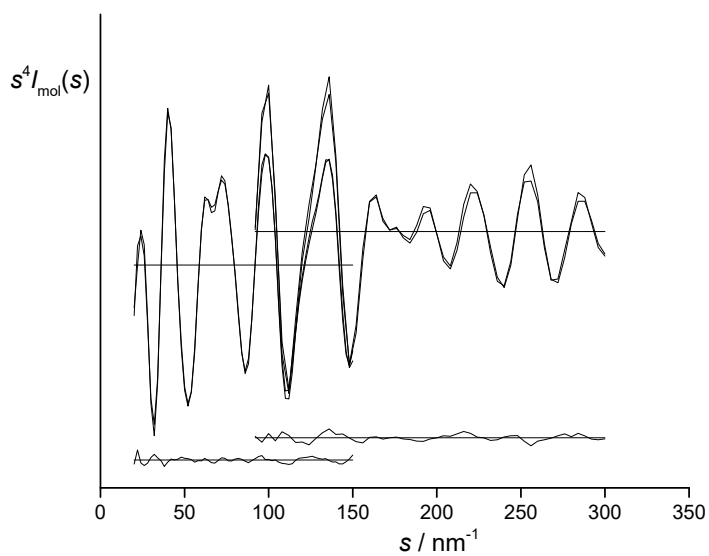


Figure S4: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for the conformer +51--.

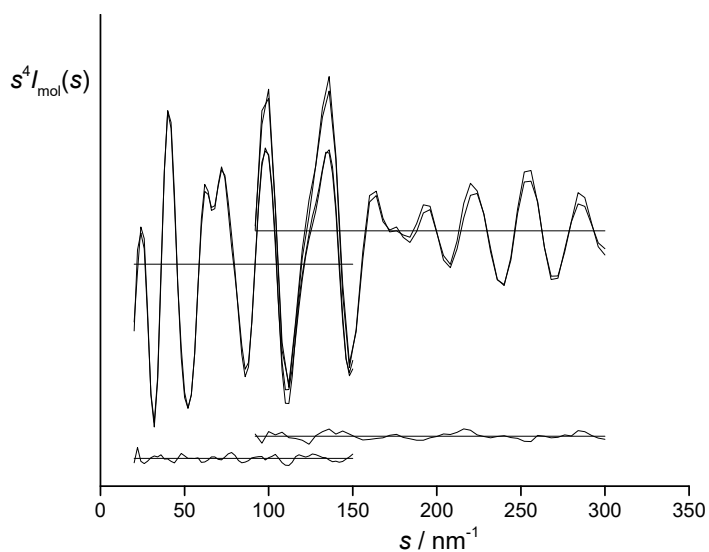


Figure S5: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for the conformer +143--.

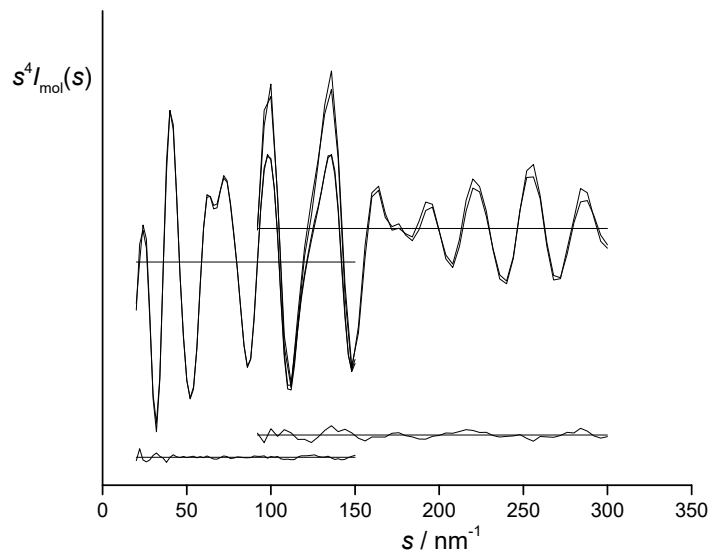


Figure S6: Experimental and final weighted difference (experimental – theoretical) molecular-scattering intensities for the combined model of +77++&+51--.

Model Construction

The model for *iso*-propyl(*tert*-butyl)(trichlorosilyl)phosphine (**1**) was constructed using 31 independent geometric parameters. On the basis of the quantum chemical calculations, all bond length of the same type are quite similar and were assumed to be equal, apart from the P-C bond length. The distances used were the average bond lengths for the Si-Cl, P-Si, C-C and C-H distances (p_1, p_2, p_4, p_5). For the P-C bond length an average (p_3) of P(1)-C(3) and P(1)-C(4) and the difference (p_{31}) were used to describe the distances where P(1)-C(3) is $p_3 + p_{31}$ and P(1)-C(4) is $p_3 - p_{31}$.

The angles for the trichlorosilyl group $\angle\text{Cl-Si-Cl}$, the *iso*-propyl group $\angle\text{H(10)-C(3)-C(9/8)}$ and the *tert*-butyl group $\angle\text{C-C-C}$ were described using one individual parameters (p_6, p_{11} , and p_{13} respectively). The $\angle\text{C-C-H}$ for each methyl group was described by one average parameter across both methyl-containing groups (p_{10}). The two $\angle\text{Si-P-C}$ were described using an average and the difference between this two angles (p_{14} and p_{15}). The *iso*-propyl angles $\angle\text{P-C-H(10)}$, $\angle\text{P-C(3)-C(8/9)}$, $\angle\text{C(8)-C(3)-C(9)}$ and the *tert*-butyl group angles $\angle\text{P-C(4)-C(11/12/13)}$ were all described by one parameter each ($p_7 - p_9, p_{12}$ and $p_{20} - p_{22}$). Also the angles $\angle\text{C-P-C}$ and $\angle\text{P-Si-Cl(5/6/7)}$ were describe by one single parameter each ($p_{15} - p_{19}$).

To define the torsion of the trichlorosilyl group the $\phi\text{Cl(6)-Si(2)-P(1)-C(3)}$ dihedral angle (p_{23}) was used. The torsions for the *iso*-propyl and *tert*-butyl groups were described by the dihedral angle $\phi\text{C(9)-C(3)-P(1)-Si(2)}$ and $\phi\text{C(11)-C(4)-P(1)-Si(2)}$ (p_{24} and p_{25}). The torsion for each methyl group was simply taken from the central phosphorus atom ($p_{26} - p_{30}$), where a positive value indicates clockwise rotation of the phosphorous atom relative to the hydrogen when viewed down the C(methyl)-C(group centre) bond.

In addition to the single conformers being refined individually, a mixed model refinement of +77++&+51-- was also undertaken. This utilised 53 independent parameters.

The bond lengths of Si-Cl, C-C and C-H are very similar for both conformers so one average distance for each parameter was used (p_1, p_4 and p_5). For the Si-P bond length the average (p_2) of both conformers and the difference (p_{31}) were necessary. To describe the P-C bond length an average of all C-P distances in both conformers was taken, the difference (p_{32}) describes the *iso*-propyl P-C(3) bond length for both conformers. The difference (p_{33}) was used to describe the *tert*-butyl P-C(4) bond length in +77++, the difference (p_{34}) was used for the other conformer.

To describe the angles for the trichlorosilyl group $\angle\text{Cl-Si-Cl}$ and $\angle\text{P-Si-Cl(6)}$, the *iso*-propyl group $\angle\text{H(10)-C(3)-C(9/8)}$ and $\angle\text{C-C-C}$, the *tert*-butyl group $\angle\text{C-C-C}$ were used one average parameter of both conformers ($p_6, p_{17}, p_{11} - p_{13}$ respectively). For the $\angle\text{C-C-H}$ angle each methyl group was described by one average parameter of both conformers and across both methyl-containing groups (p_{10}). The average angle of both conformers and a difference was used to describe the isopropyl angles $\angle\text{P-C-H(10)}$ (p_7, p_{35}), $\angle\text{P-C(3)-C(8)}$ (p_9, p_{37}), $\angle\text{P-C(3)-C(9)}$ (p_8, p_{36}), the *tert*-butyl group angles $\angle\text{P-C(4)-C(11)}$ (p_{21}, p_{42}), $\angle\text{P-C(4)-C(12)}$ (p_{22}, p_{43}), $\angle\text{P-C(4)-C(13)}$ (p_{20}, p_{41}), the trichlorosilyl group angles $\angle\text{P-Si-Cl(5)}$ (p_{18}, p_{41}), $\angle\text{P-Si-Cl(7)}$ (p_{19}, p_{42}) and $\angle\text{C-P-C}$ (p_{16}, p_{40}). The two $\angle\text{Si-P-C}$ angles of the trichlorosilyl group were described using an average of all $\angle\text{Si-P-C}$ angles in both conformers (p_{14}), the differences (p_{15}, p_{38}) to describe +77++ plus difference (p_{39}) to describe +51--. Furthermore each conformer had a unique set of torsion parameters.

Structural Distortion

The steric features of the conformers of **1** can be examined by consideration of the twist and tilt angles. The distortion of the ligands can be determined by ascertaining their tilt angles. To determine these tilt angles, centroids of the ligands have to be introduced. For the trisilyl and *tert*-butyl groups, the centres of the triangles of the Cl(5)···Cl(5)···Cl(5) and C(11)···C(12)···C(13) atoms are used to create V or W, respectively. For the construction of centroid X of the *iso*-propyl group, a point R along the C(3)–H(10) vector at a distance equivalent to the C–C distance was introduced, with the C(8)···C(9)···R triangle defining the centroid. In the same way, vectors at a distance the same as the Si–P bond length were introduced for P–C(3) and P–C(4) (auxiliary points S and T). The triangle Si···S···T gives the centroid U. The extension of the U–P vector defines the position of the lone electron pair Z on the phosphorus atom. A visualisation of the created centroids for conformer +77++ is shown in Figure S7.

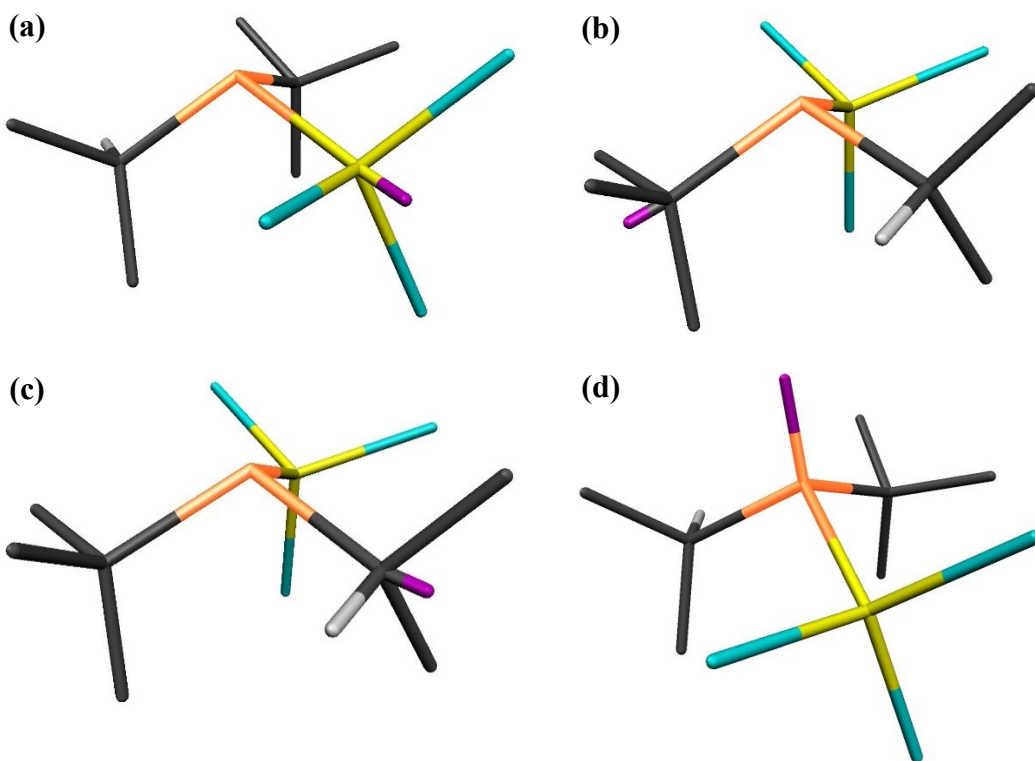


Figure S7. Representation of the constructed centroids (a) V for the SiCl₃ group, (b) W for the *tert*-butyl group, (c) X for the *iso*-propyl group and (D) Z the lone pair of electrons on the phosphorus atom. The centroids have been coloured magenta for clarity.

Having introduced the centroids, the axial tilt and the directional component can now be examined. A positive axial tilt value indicates that the group is tilted towards the lone pair of the phosphorus atom. A positive directional tilt value indicates that the torsion down Z–P–C(3)–X/ Z–P–C(4)–W and Z–P–Si–V is clockwise (positive). The axial tilt angle for the trichlorosilyl group was determined by measuring the angle between Si–P–V. C(4)–P–W describes the tilt for the *tert*-butyl group and the C(3)–P–X angle describes the axial tilt of the *iso*-propyl group. The deviation

between the perfect extensions for the centroid of each ligand was determined by measuring the S-Si-V, T-C(4)-W and U-C(3)-X angles, where S, T and U represent the extension of the P-C or P-Si bonds as shown in Figure S8. An overview of the tilt angles for the refined conformer +77++ and all the computed conformers of **1** are given in Table S16.

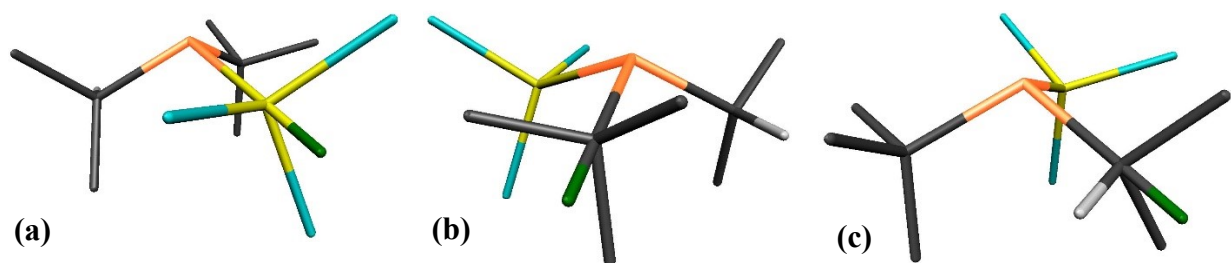


Figure S8. Representation of the constructed extensions (a) S for the SiCl_3 group, (b) T for the *tert*-butyl group and (c) U for the *iso*-propyl group. The vector extensions have been coloured green for clarity.

Table S16. Torsions and directional components for tilt angles in the five conformers of **1** computed at the B3LYP-D3/Def2TZVP level as well as the refined lowest energy structure (**R**). All values are given in degrees.

Conformer	+77++ R	+77++	+51--	-91(-)	+143--	+165+-
Tilt						
P-Si-V	1.7	1.7	1.7	1.7	1.3	1.2
P-C(4)-W	1.1	1.5	1.6	1.6	1.3	1.3
P-C(3)-X	3.4	3.1	2.9	2.9	4.7	4.6
Torsion angle from the perfectly staggered conformation						
lp-P-Si-Cl	10.5	11.5	-7.7	-0.3	-12.8	-9.5
lp-P-C-C tBu	27.0	24.7	-12.0	-4.9	-5.3	31.7
lp-P-C-H iPr	12.7	15.6	-11.2	-29.1	-37.1	-14.8
Angle between lone pair and central atom of the ligand						
lp-P-Si	125.4	124.0	125.0	127.8	125.7	125.9
lp-P-C(4)	106.5	107.0	106.8	102.5	108.7	106.9
lp-P-C(3)	107.8	107.9	105.8	108.4	108.9	111.4
Tilt direction of the ligand						
lp-P-Si-V	29.1	16.7	-4.5	24.0	-0.3	30.5
lp-P-C-W tBu	4.8	2.9	-2.0	4.3	-6.6	12.2
lp-P-C-X iPr	-88.3	-80.3	-102.6	62.5	-29.8	-11.9