Supporting Information

Reexamination of CeCl_3 and InCl_3 as Activators in the Diastereoselective Mukaiyama Aldol

Reaction in Aqueous Media.

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Experimental Section

General Information. ^1H NMR, ^{13}C NMR and ^{29}Si NMR spectra were recorded on a *VM300* (300 MHz for ^1H , 75 MHz for ^{13}C and 59.6 MHz for ^{29}Si) and *GSX400* (400 MHz for ^1H , 100 MHz for ^{13}C and 79.4 MHz for ^{29}Si). NMR spectra were recorded in CDCl_3 solution with tetramethylsilane (TMS) as an internal standard. Chemical shifts are given as δ values (ppm) and coupling constants (*J*) in Hz.

All reactions were carried out with reagent grade solvents and distilled water; reagents were used without further purification. Analytical thin layer chromatography was performed on silica gel 60-F plates; visualization was accomplished with UV light and iodine. Purification of reaction products were carried out by flash chromatography using reagent silica gel 60 (230-400 mesh). Melting points were obtained on apparatus with capillary tubes and are uncorrected.

The preparation of the silyl enolates (**Z-1** and **2**) was realized and confirmed by comparison with published data.⁹

General procedure for Mukaiyama aldol reactions catalyzed with CeCl_3 and InCl_3 .

To a solution of CeCl_3 or InCl_3 (20 mol %) in 15 mL of solvent (see Table 1) at 25 °C was added 0.15 mL (1.46 mmol, 0.156 g) of benzaldehyde with continued stirring for 30 min. Subsequently, 0.3 g (1.46 mmol) of 1-phenyl-1-(trimethyl)silyloxy-propene (**Z-1**) dissolved in 5 mL of solvent was added slowly.

The solution was stirred for 24 h at ambient temperature. The reaction was quenched by addition of 3 mL of aq. NaHCO_3 . The mixture was evaporated in a rotary evaporator and extracted with dichloromethane (3 x 40 mL), washed with 1N HCl, dried over Na_2SO_4 and concentrated. The desired product was purified by silica gel chromatography (hexane/AcOEt, 19/1).

General procedure for the desilylation of aldol products.¹⁰

To a solution of 0.2 g (0.67 mmol) of 1,3,-diphenyl-3-(trimethyl)silyloxy-propanone **3** dissolved in 15 mL of THF was added 0.76 mL (0.76 mmol) of sol. aqueous 1N of tetrabutylammonium fluoride and stirred for 30 min. Then the mixture was evaporated in a rotary evaporator and extracted with dichloromethane (3 x 40 mL), washed with 1N HCl, dried over Na_2SO_4 , and concentrated. The desired product was purified by silica gel chromatography (hexane/AcOEt, 19/1).

1-Phenyl-1-(trimethyl)silyloxy-propene (Z-1). This compound was prepared and purified according to the procedure described by House et al.⁹ bp 56-58 °C/1 mm Hg (lit.⁹ bp 89-91 °C/12 mm Hg). ^1H NMR (CDCl_3) δ 0.19 (s, 9H), 1.79 (d, 3H, $J = 6.9$ Hz), 5.38 (q, 1H, $J = 6.9$ Hz), 7.31-7.51 (m, 5H); ^{13}C NMR (CDCl_3) δ 0.61, 11.71, 105.34, 125.24, 127.31, 128.04, 139.24, 149.92; ^{29}Si NMR (CDCl_3) δ 19.46.

1-Phenyl-1-(trimethyl)silyloxy-ethene (2). This compound was prepared and purified according to the procedure described by House et al.⁹ bp 95 °C/2 mm Hg, (lit.^{9b} bp 117-119 °C/26-28 mm Hg). ^1H NMR (CDCl_3) δ 0.33 (s, 9H), 4.50 (d, 1H, $J = 1.8$ Hz), 4.90 (d, 1H, $J = 1.5$ Hz), 7.26-7.66 (m, 5H); ^{13}C NMR (CDCl_3) δ 0.16, 91.12, 125.26, 128.13, 128.28, 137.55, 155.69; ^{29}Si NMR (CDCl_3) δ 19.40.

1,3-Diphenyl-3-trimethylsilyloxy-propanone (3).¹¹ ^1H NMR (CDCl_3) δ 0.01 (s, 9H), 3.03 (dd, 1H, $J = 3.8$ Hz, 15.3 Hz), 3.58 (dd, 1H, $J = 8.9$ Hz, 15.5 Hz), 5.41 (dd, 1H, $J = 3.6$ Hz, 8.8 Hz), 7.24-7.88 (m,

10H); ^{13}C NMR (CDCl_3) δ 0.07, 26.6, 71.70, 125.77, 127.37, 128.37, 128.42, 128.49, 132.99, 137.61, 144.76, 198.40; ^{29}Si NMR (CDCl_3) δ 18.30.

3-Hidroxy-1,3-diphenyl-propanone (4).¹¹ mp 52 °C, (lit.¹¹ mp 52-53 °C). ^1H NMR (CDCl_3) δ 3.36 (dd, 2H, $J = 3.9$ Hz, 8.8 Hz), 3.78-4.01 (bs, 1H), 5.35 (dd, 1H, $J = 3.5$ Hz, 8.3 Hz), 7.29-7.96 (m, 10H); ^{13}C NMR (CDCl_3) δ 47.49, 70.05, 125.84, 127.69, 128.24, 128.59, 128.73, 133.65, 136.63, 143.15, 200.10.

syn-**3-Hidroxy-2-methyl-1,3-diphenyl-propanone (5).**¹¹ ^1H NMR (CDCl_3) δ 1.20 (d, 3H, $J = 6.9$ Hz), 3.70 (m, 1H), 5.22 (d, 1H, $J = 3.1$ Hz) 7.23-7.98 (m, 10H); ^{13}C NMR (CDCl_3) δ 14.10, 47.44, 73.48, 126.13, 126.90, 128.08, 128.52, 128.81, 133.47, 135.78, 141.99, 205.36.

anti-**3-Hidroxy-2-methyl-1,3-diphenyl-propanone (5).**¹¹ ^1H NMR (CDCl_3) δ 1.05 (d, 3H, $J = 7.3$ Hz), 3.84 (q, 1H, $J = 7.4$ Hz), 4.98 (d, 1H, $J = 8.1$ Hz) 7.34-7.85 (m, 10H); ^{13}C NMR (CDCl_3) δ 15.60, 48.09, 75.83, 126.21, 127.47, 128.40, 128.62, 128.94, 133.73, 136.88, 142.35, 204.91.

3-Hidroxy-2-methyl-3-(4-nitro-phenyl)-1-phenyl-propanone (6).¹¹ ^1H NMR (CDCl_3) δ 1.09 (d, 3H, $J = 7.3$ Hz), 1.14 (d, 3H, $J = 7.3$ Hz), 3.70 (m, 1H), 3.82 (q, 1H, $J = 7.3$ Hz), 4.09 (bs, 1H), 5.08 (d, 1H, $J = 7.3$ Hz), 5.33 (d, 1H, $J = 2.5$ Hz), 7.45-8.19 (m, 18H).; ^{13}C NMR (CDCl_3) δ 11.0, 46.5, 72.3, 123.5, 126.9, 128.5, 128.9 133.9, 135.1, 147.2, 149.2, 205.2.

3-Hidroxy-3-(4-methoxy-phenyl)-2-methyl-1-phenyl-propanone (7).¹¹ ^1H NMR (CDCl_3) δ 1.04 (d, 3H, $J = 7.3$ Hz), 1.21 (d, 3H, $J = 7.3$ Hz), 2.86 (bs, 1H), 3.51 (bs, 1H), 3.68 (m, 2H), 3.80 (d, 6H, $J = 5.1$ Hz), 4.95 (d, 1H, $J = 8.4$ Hz), 5.18 (d, 1H, $J = 3.6$ Hz), 6.87-7.98 (m, 18H).; ^{13}C NMR (CDCl_3) δ 11.4,

15.7, 47.2, 48.1, 55.2, 55.5, 72.9, 76.4, 113.6, 113.8, 114.3, 127.2, 127.9, 128.4, 128.6, 128.7, 131.9, 133.2, 133.5, 190.7, 190.8.

3-(4-Chloro-phenyl)-3-hydroxy-2-methyl-1-phenyl-propanone (8).¹¹ ¹H NMR (CDCl₃) δ 1.03 (d, 3H, J = 6.9 Hz), 1.16 (d, 3H, J = 7.3 Hz), 3.46 (bs, 1H), 3.64 (m, 1H), 3.77 (q, 1H, J = 7.3 Hz), 3.91 (bs, 1H), 4.94 (d, 1H, J = 8.0 Hz), 5.17 (d, 1H, J = 3.3 Hz), 7.27-7.96 (m, 18H).; ¹³C NMR (CDCl₃) δ 11.3, 15.6, 47.0, 47.9, 72.6, 75.9, 127.5, 128.1, 128.3, 128.4, 128.5, 128.7, 128.8, 133.4, 135.5, 136.6, 140.4, 140.8, 204.7, 205.4.

3-hydroxy-2-methyl-1-phenyl-butanone (9).¹⁸ ¹H NMR (CDCl₃) δ 1.21 (d, 3H, J = 6.9 Hz), 1.27 (d, 3H, J = 6.9 Hz), 2.73 (bs, 1H), 3.44 (m, 1H), 4.31 (m, 1H), 7.25-7.63 (m, 5H); ¹³C NMR (CDCl₃) δ 12.1, 15.6, 20.9, 21.3, 46.7, 48.3, 68.2, 70.3, 129.1, 129.3, 133.9, 134.0, 136.9, 137.4, 205.8, 205.9.

3-hydroxy-2,4-dimethyl-1-phenyl-pentanone (10).¹¹ ¹H NMR (CDCl₃) δ 0.99 (m, 12H), 1.26 (dd, 6H, J = 7.3 Hz, J = 6.9 Hz), 1.79 (m, 2H), 3.67 (m, 4H), 7.48-7.98 (m, 10H).; ¹³C NMR (CDCl₃) δ 16.0, 17.0, 19.1, 20.0, 30.8, 31.3, 41.9, 42.4, 77.0, 79.2, 129.3, 128.5, 128.8, 133.4, 205.6, 205.9.

3-hydroxy-2,4,4-trimethyl-1-phenyl-pentanone (11).¹¹ ¹H NMR (CDCl₃) δ 0.88 (s, 9H), 0.98 (s, 9H), 1.46 (d, 3H, J = 6.9 Hz), 1.68 (d, 3H, J = 6.9 Hz), 3.65 (m, 2H), 3.78 (m, 2H), 7.39-7.95 (m, 10H).; ¹³C NMR (CDCl₃) δ 13.1, 26.9, 40.9, 77.5, 99.9, 128.5, 128.8, 133.3, 205.3.

The absolute energy values, imaginary frequencies and relative energies for intermediates **I-VIII** are collected in Table 5. The Cartesian coordinates obtained for these intermediates at B3LYP/LANL2DZ level are showed below. The geometries obtained at PM3, HF/3-21G* and B3LYP/3-21G* are not included because differences with B3LYP/LANL2DZ results are not significant.

Table 5. Calculated imaginary frequencies, absolute and relative energies for “open” InCl₃-promoted transition states leading to *anti*-**5** (**I-III**) and *syn*-**5** (**IV-VI**). See Scheme 3.

	PM3	HF/3-21G*	B3LYP/3-21G*	B3LYP/LANL2DZ
	E_{abs} (kcal/mol)/[freq]	E_{abs} (Hartrees)	E_{abs} (Hartrees)	E_{abs} (Hartrees)
	E_{rel} (kcal/mol)	E_{rel} (kcal/mol)	E_{rel} (kcal/mol)	E_{rel} (kcal/mol)
I	-147.145/[254.38i] 6.313	-8253.4697410 4.597	-8264.4277858 6.115	-939.6194178 14.940
II	-149.355/[259.37i] 4.103	-8253.4725703 2.822	-8264.4294321 5.082	-939.6323343 6.835
III	-144.654/[239.06i] 8.804	-8253.4647946 7.701	-8264.4174525 12.599	-939.6283674 9.324
IV	-145.699/[253.61i] 7.759	-8253.4656296 7.177	-8264.4195385 11.290	-939.6234576 12.405
V	-153.458/[255.14i] 0.000	-8253.4770681 0.000	-8264.4375311 0.000	-939.6432271 0.000
VI	-150.403/[258.09i] 3.055	-8253.4607274 10.253	-8264.4292785 5.178	-939.6256838 11.008
VII	-164.098/[175.59i] 0.000	-8253.489406 0.000	-8264.458912 0.000	-939.5806672 0.000
VIII	-158.559/[183.37i] 5.539	-8253.4803718 5.669	-8264.4479012 6.909	-939.5728755 4.889

Cartesian coordinates for intermediates **I-VIII** at B3LYP/LANL2DZ level of theory.

		Cartesian Coordinates (Angstroms)		
Atom		X	Y	Z
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1	H H1	4.5223845	0.0394719	3.6812598
2	C C1	3.6528199	0.3068312	4.2958991
3	C C2	1.4936010	1.0032779	5.9064451
4	C C3	3.0409754	1.5497437	4.1280102
5	C C4	3.1820772	-0.5820945	5.2578916
6	C C5	2.1014789	-0.2383236	6.0614445
7	C C6	1.9615627	1.8926923	4.9472328
8	H H3	3.6733649	-1.5521025	5.3874060
9	H H4	1.7372501	-0.9362819	6.8219191
10	H H5	1.4910423	2.8787755	4.8486392
11	H H6	0.6547895	1.2860183	6.5503127
12	C C7	3.5365433	2.5615980	3.0991569
13	H H10	3.2437893	3.5902525	3.4430199
14	O O1	4.8871002	2.4482064	2.9184214
15	C C8	2.7838123	2.3242683	1.7037995
16	H H11	3.1963376	3.1563876	1.0376916
17	C C9	3.1019419	0.9720412	1.0871812
18	H H8	2.4625992	0.7452645	0.2157532
19	H H13	2.9666119	0.1543519	1.8104967
20	H H14	4.1482719	0.9410777	0.7550101
21	C C10	1.3194790	2.5818987	1.8151313
22	C C11	0.7852405	3.9290163	2.0345534
23	C C12	-0.1813932	6.5056199	2.4732277
24	C C13	1.4767777	5.0346345	1.5247201
25	C C14	-0.3940503	4.1229399	2.7719193
26	C C15	-0.8673231	5.4065133	2.9917453
27	C C16	0.9841117	6.3179904	1.7398899
28	H H12	2.4256150	4.8782863	0.9640177
29	H H17	-0.9304704	3.2609155	3.1924532
30	H H18	-1.7782621	5.5594330	3.5809601
31	H H19	1.5337301	7.1794881	1.3408617
32	H H20	-0.5599521	7.5184432	2.6529001
33	O O2	0.5525633	1.5764902	1.6990777
34	Si Si1	-0.9681989	1.1684147	0.9857555
35	C C17	-0.3399673	-0.1302234	-0.2247562
36	H H15	-0.6321744	-1.1412733	0.0735001
37	H H23	0.7621309	-0.1019999	-0.2729183

38	H	H24	-0.7205156	0.0488188	-1.2349547
39	C	C18	-2.0138614	0.4878933	2.3798452
40	H	H16	-2.9348884	0.0448178	1.9836899
41	H	H25	-2.3016121	1.2669444	3.0936123
42	H	H26	-1.4853545	-0.2940456	2.9353041
43	C	C19	-1.7714570	2.6158582	0.1080612
44	H	H21	-2.7451297	2.3097115	-0.2926543
45	H	H27	-1.1686019	2.9711345	-0.7336498
46	H	H28	-1.9422884	3.4652832	0.7788133
47	In	In1	5.9016503	4.2074215	2.4845761
48	Cl	Cl1	5.2382993	5.8643442	4.0543398
49	Cl	Cl2	8.1717264	3.7934162	2.1597594
50	Cl	Cl3	4.7033572	4.8402167	0.3158883

			Cartesian Coordinates (Angstroms)		
Atom			X	Y	Z

1	C	C7	-0.2118765	-3.6502323	1.7933054
2	C	C8	1.3479523	-3.9321634	1.4956189
3	H	H11	1.7054123	-4.6468672	2.2903199
4	C	C9	1.4755451	-4.6304337	0.1524859
5	H	H8	2.5031810	-4.9624876	-0.0421901
6	H	H13	1.1649712	-3.9891812	-0.6867144
7	H	H14	0.8250790	-5.5244010	0.1452502
8	C	C10	2.2266901	-2.7246912	1.6388193
9	C	C11	2.7300813	-2.3171123	2.9640315
10	C	C12	3.6789401	-1.5738653	5.4841999
11	C	C13	2.8392678	-3.2664654	3.9908903
12	C	C14	3.0942324	-0.9880732	3.2189491
13	C	C15	3.5637903	-0.6232732	4.4748214
14	C	C16	3.3168111	-2.8963895	5.2394677
15	H	H12	2.5325214	-4.3077127	3.8005872
16	H	H17	2.9859310	-0.2201678	2.4319801
17	H	H18	3.8338331	0.4203813	4.6717671
18	H	H19	3.3992412	-3.6449876	6.0353553
19	H	H20	4.0478634	-1.2817038	6.4737729
20	O	O2	2.6921005	-2.1373123	0.6288912
21	Si	Si1	2.6941045	-0.9533901	-0.6249937
22	C	C17	4.5021245	-0.9942675	-1.1415553
23	H	H15	4.6741999	-0.2494432	-1.9277345
24	H	H23	4.7938543	-1.9699987	-1.5414233

25	H	H24	5.1730732	-0.7575890	-0.3101009
26	C	C18	1.5491889	-1.5454653	-1.9729652
27	H	H16	1.4870678	-0.7873123	-2.7636456
28	H	H25	0.5243756	-1.7146986	-1.6047890
29	H	H26	1.8993845	-2.4760543	-2.4307598
30	C	C19	2.2227345	0.6767710	0.1607001
31	H	H21	2.4436674	1.4995714	-0.5285076
32	H	H27	2.7837678	0.8559766	1.0887876
33	H	H28	1.1516102	0.7296456	0.4082144
34	H	H32	-0.7572019	-3.7780983	0.8182356
35	O	O1	-0.3890234	-2.3924521	2.2982234
36	C	C1	-0.6229456	-4.7768567	2.7409678
37	C	C2	-1.3471401	-6.9185890	4.3830334
38	C	C3	-0.7254509	-6.0708300	2.2169689
39	C	C4	-0.8765567	-4.5687456	4.0953763
40	C	C5	-1.2401632	-5.6377564	4.9108412
41	C	C6	-1.0867219	-7.1345189	3.0324212
42	H	H3	-0.4998324	-6.2346643	1.1505983
43	H	H4	-0.8036213	-3.5588456	4.5184436
44	H	H5	-1.4502256	-5.4632754	5.9712874
45	H	H6	-1.1715577	-8.1419567	2.6125865
46	H	H7	-1.6395945	-7.7553654	5.0255156
47	In	In1	-1.9804901	-1.2883412	1.5139891
48	Cl	Cl1	-4.0494516	-1.6012901	2.5412762
49	Cl	Cl2	-1.8528576	-2.0141878	-0.8465456
50	Cl	Cl3	-1.0237856	0.9174443	1.6596678

			Cartesian Coordinates (Angstroms)		
Atom			X	Y	Z
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1	C	C7	-0.3122399	-4.8720660	2.1588562
2	C	C8	1.2687164	-5.1211805	2.1288564
3	H	H11	1.4777958	-5.6831483	3.0796825
4	C	C9	1.5901232	-6.0121684	0.9386943
5	H	H8	2.6607724	-6.2431147	0.8658321
6	H	H13	1.2751002	-5.5307016	-0.0075239
7	H	H14	1.0562618	-6.9691556	1.0157680
8	C	C10	2.1760991	-3.9297776	2.2278748
9	C	C11	2.3262781	-3.1766234	3.4935007
10	C	C12	2.6533325	-1.7736815	5.8707234
11	C	C13	2.8708987	-3.8171834	4.6113703

12	C	C14	1.9273873	-1.8404645	3.5697578
13	C	C15	2.0956007	-1.1445255	4.7636682
14	C	C16	3.0391884	-3.1101324	5.7940851
15	H	H12	3.1642069	-4.8722380	4.5571993
16	H	H17	1.4500798	-1.3511977	2.6977623
17	H	H18	1.7751474	-0.0983837	4.8271949
18	H	H19	3.4681469	-3.6082076	6.6704630
19	H	H20	2.7821234	-1.2215922	6.8082762
20	O	O2	2.9081116	-3.6564749	1.2404430
21	Si	Si1	4.2037742	-2.5534567	0.8564455
22	C	C17	4.5408689	-3.0742353	-0.9113989
23	H	H15	5.0039997	-2.2537963	-1.4701945
24	H	H23	3.6022457	-3.3353357	-1.4259254
25	H	H24	5.2056618	-3.9404804	-0.9685996
26	C	C18	3.6662456	-0.7693632	0.9930241
27	H	H16	4.3063390	-0.1371267	0.3673857
28	H	H25	3.7213578	-0.3941678	2.0197007
29	H	H26	2.6295787	-0.6366469	0.6432988
30	C	C19	5.6081234	-2.9814977	2.0300478
31	H	H21	6.4565456	-2.3118256	1.8471313
32	H	H27	5.9637884	-4.0065206	1.8890200
33	H	H28	5.3195590	-2.8668567	3.0797588
34	H	H36	-0.7228529	-5.9211943	2.1251367
35	O	O1	-0.9437567	-4.2383357	1.1548435
36	C	C1	-0.6943725	-4.2968591	3.5235207
37	C	C2	-1.5358017	-3.3760118	6.0243359
38	C	C3	-0.7137324	-5.1565268	4.6262254
39	C	C4	-1.1018871	-2.9731445	3.6851329
40	C	C5	-1.5244170	-2.5181701	4.9311343
41	C	C6	-1.1265567	-4.6970164	5.8701997
42	H	H3	-0.4202440	-6.2064322	4.5075926
43	H	H4	-1.0979872	-2.2931554	2.8171999
44	H	H5	-1.8562045	-1.4808508	5.0448997
45	H	H6	-1.1425234	-5.3784567	6.7266982
46	H	H7	-1.8736947	-3.0175191	7.0017455
47	In	In1	-0.7112560	-3.1857055	-0.5602569
48	Cl	Cl1	0.1936676	-1.1188567	0.5974307
49	Cl	Cl2	1.1114432	-3.9191779	-1.9605453
50	Cl	Cl3	-2.8084549	-2.9935789	-1.4998567

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
1	H	H1	3.9491678	-3.4897864	-0.0501551
2	C	C1	3.1838778	-4.1840340	0.3201174
3	C	C2	1.2977597	-5.9916789	1.2759651
4	C	C3	2.8873715	-4.2153123	1.6840530
5	C	C4	2.5372878	-5.0480333	-0.5577989
6	C	C5	1.5890206	-5.9481602	-0.0831765
7	C	C6	1.9506528	-5.1363078	2.1568699
8	H	H3	2.7862875	-5.0274392	-1.6239913
9	H	H4	1.0862123	-6.6325898	-0.7740318
10	H	H5	1.7440383	-5.2069603	3.2331021
11	H	H6	0.5689884	-6.7137246	1.6591567
12	C	C7	3.5952456	-3.2786418	2.6670718
13	H	H10	3.3687780	-3.5849765	3.7218209
14	O	O1	4.9286995	-3.2209024	2.3948321
15	C	C8	2.9608445	-1.8179243	2.4552330
16	H	H9	3.2439271	-1.4809290	1.4252716
17	C	C9	3.5166567	-0.8330018	3.4725705
18	H	H8	3.3054376	0.2042789	3.1831243
19	H	H13	4.6135620	-0.9586720	3.5513432
20	H	H14	3.1242819	-0.9991252	4.4874806
21	C	C10	1.4641477	-1.8612565	2.5361456
22	O	O2	0.9327789	-2.2203288	3.6199036
23	C	C11	0.6696555	-1.4543535	1.36049435
24	C	C12	-0.7379512	-0.6615438	-0.9028372
25	C	C13	-0.2362879	-2.3338678	0.7619356
26	C	C14	0.8831801	-0.1834451	0.8155638
27	C	C15	0.1681730	0.2123134	-0.3076157
28	C	C16	-0.9340856	-1.9335991	-0.3722174
29	H	H15	-0.3713465	-3.3477456	1.1664099
30	H	H17	1.6159433	0.4941982	1.2745456
31	H	H18	0.3277678	1.2108246	-0.7307186
32	H	H19	-1.6338104	-2.6267757	-0.8528517
33	H	H20	-1.2913567	-0.3501239	-1.7961827
34	Si	Si1	-0.6496150	-2.5201567	4.2781436
35	C	C17	-0.3690710	-2.0766220	6.0747654
36	H	H12	-1.1603216	-2.5066084	6.6996784
37	H	H23	-0.3699421	-0.9941502	6.2357899
38	H	H24	0.5873765	-2.4661419	6.4423432

39	C	C18	-0.9467962	-4.3529102	4.0194453
40	H	H21	-1.9702321	-4.6160109	4.3094535
41	H	H25	-0.2652440	-4.9562432	4.6299135
42	H	H26	-0.8069168	-4.6599799	2.9759342
43	C	C19	-1.9611967	-1.4442432	3.4845479
44	H	H16	-2.9242903	-1.6131108	3.9816474
45	H	H27	-2.0970432	-1.6664432	2.4199758
46	H	H28	-1.7302548	-0.3780342	3.5758801
47	In	In1	6.2344832	-3.5599678	3.9794043
48	Cl	Cl1	5.1432432	-2.3394879	5.8542150
49	Cl	Cl2	8.3074456	-2.6437564	3.3380189
50	Cl	Cl3	6.2228632	-5.8804778	4.4809701

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z
1 C C1	1.0694874	-1.8169963	0.8634840
2 H H4	0.7180862	-2.3462432	1.7870360
3 C C2	0.2801289	-2.3341567	-0.3394042
4 C C3	-1.2460198	-3.2512743	-2.4935464
5 C C4	-1.0153765	-2.8194034	-0.1340333
6 C C5	0.8049453	-2.3166392	-1.6318895
7 C C6	0.0429739	-2.7750543	-2.7032765
8 C C7	-1.7736206	-3.2745643	-1.2057781
9 H H6	-1.4329072	-2.8547789	0.8792681
10 H H7	1.8273983	-1.9542415	-1.8015350
11 H H8	0.4656170	-2.7653125	-3.7135999
12 H H9	-2.7842420	-3.6600321	-1.0352612
13 H H10	-1.8426876	-3.6140225	-3.3371109
14 O O1	2.4232906	-1.8850456	0.7171699
15 C C8	0.6080059	-0.2795291	1.0044899
16 H H12	-0.4981049	-0.2835022	0.8081121
17 C C9	1.2801873	0.6216343	-0.0130644
18 H H2	0.8895167	1.6464078	0.0348013
19 H H13	1.0982365	0.2392876	-1.0282610
20 H H14	2.3696441	0.6670532	0.1224332
21 C C10	0.7554664	0.1915567	2.4194105
22 C C11	-0.2484543	-0.2290175	3.4211222
23 C C12	-2.1777543	-1.0544243	5.2486971
24 C C13	0.1277772	-0.9802456	4.5365458
25 C C14	-1.5938612	0.1016053	3.2159762
26 C C15	-2.5508543	-0.3036535	4.1353919

27	C	C16	-0.8442354	-1.3934758	5.4438884
28	H	H11	1.1883831	-1.2749765	4.6862183
29	H	H17	-1.8939795	0.6813380	2.3339780
30	H	H18	-3.6028459	-0.0399491	3.9798543
31	H	H19	-0.5489465	-1.9979654	6.3094260
32	H	H20	-2.9387102	-1.3826744	5.9657922
33	O	O2	1.6892323	0.9878357	2.7050622
34	Si	Si1	2.1988893	1.8667961	4.1213389
35	C	C17	3.5319324	2.9515789	3.3701232
36	H	H16	3.1528396	3.5582042	2.5423543
37	H	H23	4.3663543	2.3515239	2.9904173
38	H	H24	3.9336735	3.6352543	4.1274451
39	C	C18	0.7245526	2.8672500	4.7170012
40	H	H21	0.2014095	3.3704654	3.8980384
41	H	H25	1.0651851	3.6437916	5.4121810
42	H	H26	-0.0043765	2.2454193	5.2478654
43	C	C19	2.8676334	0.7073228	5.4221129
44	H	H22	3.4173861	1.2666987	6.1868196
45	H	H27	3.5583941	-0.0306325	4.9835543
46	H	H28	2.0735596	0.1399509	5.9224654
47	In	In1	3.4516281	-3.3630785	1.7506211
48	Cl	Cl1	5.6809976	-3.2765424	1.0391781
49	Cl	Cl2	2.3660765	-5.4485065	1.8010019
50	Cl	Cl3	3.2164263	-2.3128976	4.0578456

			Cartesian Coordinates (Angstroms)		
Atom			X	Y	Z
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1	C	C20	1.2808543	0.0725624	2.0465905
2	C	C8	2.4792106	0.3238435	1.0094456
3	C	C10	3.3910693	1.4505549	1.3712638
4	H	H31	0.9502252	-0.9868854	1.8594246
5	C	C1	1.7670006	0.1589262	3.4895172
6	C	C2	2.5488556	0.2119780	6.1752154
7	C	C3	2.2275543	-1.0019561	4.1177551
8	C	C4	1.6921654	1.3434974	4.2240873
9	C	C5	2.0801789	1.3679658	5.5603282
10	C	C6	2.6217421	-0.9734003	5.4508866
11	H	H2	2.2569543	-1.9492204	3.5637765

12	H	H3	1.2924543	2.2512978	3.7539377
13	H	H4	1.9976543	2.2974897	6.1333848
14	H	H5	2.9729643	-1.8907092	5.9349999
15	H	H6	2.8431306	0.2304499	7.2294543
16	O	O1	0.2639685	0.9613543	1.8270628
17	In	In1	-1.1986765	0.3096227	0.4905037
18	Cl	Cl1	-1.3626187	-2.0536017	0.6854065
19	Cl	Cl2	0.1068653	0.8707065	-1.5941540
20	Cl	Cl3	-3.1367896	1.5989838	0.6995094
21	H	H1	1.9437987	0.6400876	0.0517276
22	C	C7	3.2246767	-0.9749477	0.7512487
23	H	H8	3.6492845	-1.3993168	1.6739512
24	H	H9	4.0476765	-0.8364876	0.0374196
25	H	H10	2.5496188	-1.7301962	0.3244676
26	C	C9	3.0375432	2.8518631	1.1125201
27	C	C17	2.3986278	5.5098543	0.5493558
28	C	C18	3.5702084	3.8899554	1.8955432
29	C	C19	2.1766432	3.1613287	0.0505257
30	C	C21	1.8683231	4.4888432	-0.2295453
31	C	C22	3.2466472	5.2071623	1.6153432
32	H	H11	4.2325854	3.6582543	2.7468957
33	H	H13	1.7288578	2.3409493	-0.5518639
34	H	H14	1.1920760	4.7205432	-1.0614847
35	H	H15	3.6537181	6.0135226	2.2350657
36	H	H16	2.1467322	6.5540818	0.3321303
37	O	O2	4.5756099	1.2308432	1.7625684
38	Si	Si1	5.7521124	0.9122866	2.9685931
39	C	C11	5.3651719	2.0422793	4.4155133
40	H	H12	6.2159456	2.0761244	5.1046075
41	H	H20	4.4884949	1.6965430	4.9801716
42	H	H21	5.1622755	3.0696310	4.0820869
43	C	C12	5.6926832	-0.9012256	3.4241432
44	H	H19	6.482546	-1.1277743	4.1496999
45	H	H22	5.8467781	-1.5472792	2.5536675
46	H	H23	4.7321567	-1.1748564	3.8823161
47	C	C13	7.3422535	1.3771190	2.0860456
48	H	H17	8.1912740	1.2803351	2.7730654
49	H	H24	7.3229168	2.4101654	1.7252428
50	H	H25	7.5341743	0.7261907	1.2272756

Cartesian Coordinates (Angstroms)

Atom		X	Y	Z
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1	C C1	-2.1270490	0.4020018	2.9002910
2	C C2	0.3735434	-0.0828547	2.8330085
3	O O1	0.8642873	1.0695543	2.7759888
4	O O2	-1.8934872	1.7606324	2.9382844
5	C C6	-0.9616395	-0.3693543	2.1770864
6	H H12	-1.1779549	-1.4611661	2.3037497
7	In In1	-0.9620676	2.4228655	4.6610447
8	Cl Cl1	-1.0695594	0.5325534	6.2437774
9	Cl Cl2	1.5962260	2.7685678	4.6204472
10	Cl Cl3	-1.8359180	4.4744543	5.3160473
11	Si Si1	2.5392456	1.6561945	2.5654122
12	C C3	3.8744024	0.9199759	3.6822313
13	H H10	4.8548194	1.0388562	3.2091672
14	H H15	3.7060117	-0.1489623	3.8479771
15	H H16	3.9059368	1.4154114	4.6576710
16	C C4	2.7068878	0.7528566	0.8635395
17	H H13	2.7240828	-0.3398555	0.9460775
18	H H17	3.6567840	1.0714345	0.4223367
19	H H18	1.9069695	1.0256347	0.1692976
20	C C5	2.8159008	3.4590134	2.0386576
21	H H14	3.0886096	4.0979589	2.8834491
22	H H19	1.9175654	3.8764407	1.5751892
23	H H20	3.6254014	3.4969180	1.3022586
24	C C7	-0.8658654	-0.0711655	0.6880645
25	H H9	-0.0441012	-0.6317653	0.2205654
26	H H21	-0.7012837	0.9968654	0.4873952
27	H H22	-1.8005429	-0.3552287	0.1844654
28	C C8	1.0625412	-1.2387136	3.4673555
29	C C9	2.2447911	-3.4722807	4.6220063
30	C C10	0.7968653	-1.5480974	4.8020554
31	C C11	1.9151490	-2.0445337	2.7091245
32	C C12	2.5039350	-3.1600443	3.2899131
33	C C13	1.3960059	-2.6670295	5.3730435
34	H H6	0.1132452	-0.8985374	5.4113454
35	H H23	2.1261793	-1.7875677	1.6590780
36	H H24	3.1725903	-3.7933938	2.6972296
37	H H25	1.1922995	-2.9091175	6.4223319
38	H H26	2.7109437	-4.3529934	5.0770764

39	H	H5	-2.2060645	-0.0307669	3.9370496
40	C	C14	-3.4263282	0.0851049	2.1729817
41	C	C15	-5.8191477	-0.5807543	0.8950784
42	C	C16	-3.9716952	0.9378122	1.2131147
43	C	C17	-4.0896990	-1.1044543	2.4885724
44	C	C18	-5.2784704	-1.4355289	1.8504522
45	C	C19	-5.1655338	0.6045745	0.5800769
46	H	H3	-3.4653676	1.8782855	0.9637435
47	H	H4	-3.6757556	-1.7778036	3.2484541
48	H	H7	-5.7932133	-2.3675174	2.1052096
49	H	H8	-5.5918327	1.2828690	-0.1662757
50	H	H11	-6.7589683	-0.8395012	0.3970444

			Cartesian Coordinates (Angstroms)		
Atom			X	Y	Z
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1	C	C2	1.7840658	0.8838059	0.9567107
2	C	C8	3.2935462	0.7733746	0.5467340
3	C	C10	3.9723355	2.1064875	0.2874840
4	Cl	Cl1	1.3315422	4.4433426	-1.1161547
5	Cl	Cl2	3.0082599	5.2232843	2.1041601
6	Cl	Cl3	-0.8017897	4.5399442	2.3010200
7	C	C7	4.0760769	0.0223772	1.6195855
8	H	H2	4.0001090	0.5105427	2.6012113
9	H	H9	5.1434389	-0.0507493	1.3647531
10	H	H10	3.6925767	-1.0006913	1.7310542
11	H	H15	3.3448429	0.1782099	-0.4060789
12	C	C13	4.6833580	2.2582780	-1.0096439
13	C	C14	6.0041523	2.4772735	-3.4555486
14	C	C15	4.4519987	3.3622367	-1.8327212
15	C	C16	5.5802084	1.2624959	-1.4180569
16	C	C17	6.2401543	1.3775922	-2.6330999
17	C	C18	5.1110435	3.4632866	-3.0553553
18	H	H11	3.7235113	4.1380765	-1.5381326
19	H	H14	5.7731483	0.3967325	-0.7711767
20	H	H16	6.9458175	0.6004769	-2.9461547
21	H	H21	4.9163912	4.3262484	-3.7023803
22	H	H23	6.5212879	2.5615530	-4.4176697
23	O	O2	3.9744672	2.9928904	1.1732929

24	In	In1	1.1036623	3.6835147	1.1940550
25	Si	Si1	5.2235383	4.1460348	1.7441835
26	C	C9	5.3611122	4.4369571	3.6183748
27	H	H12	6.3770987	4.2175886	3.9597749
28	H	H18	4.6702671	3.7890603	4.1665033
29	H	H19	5.1232534	5.4726330	3.8750733
30	C	C11	5.6679735	5.6229240	0.6443923
31	H	H17	5.6062056	5.3560646	-0.4158967
32	H	H20	6.6933637	5.9428568	0.8552546
33	H	H22	5.0012010	6.4723749	0.8215334
34	C	C12	6.6682624	2.8877219	1.4691476
35	H	H13	7.5737548	3.3568364	1.8682925
36	H	H24	6.8467293	2.6552647	0.4155984
37	H	H25	6.5144617	1.9466890	2.0050357
38	C	C19	0.8443122	1.0710469	-0.2277325
39	C	C21	-1.0037534	1.1758446	-2.3393294
40	C	C22	-0.4608474	1.5325925	-0.0063121
41	C	C23	1.1906075	0.6285945	-1.5128274
42	C	C24	0.2820837	0.6872788	-2.5589395
43	C	C25	-1.3722121	1.5873817	-1.0665242
44	H	H7	-0.8437322	1.7324905	1.0112768
45	H	H26	2.1946203	0.2204446	-1.6993575
46	H	H27	0.5756567	0.3467915	-3.5573101
47	H	H28	-2.3903785	1.9496657	-0.8839601
48	H	H29	-1.7202491	1.2264645	-3.1655921
49	H	H8	1.5131456	-0.0884776	1.4473690
50	O	O1	1.5977765	1.8233745	1.9445557