Electronic supplementary information

for

Flexibility and lability of a phenyl ligand in hetero-organometallic 3d metal-Sn(IV) compounds and their catalytic activity towards Baeyer–Villiger oxidation of cyclohexanone

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Structural scarcity of related organometallic compounds

A search for the Co–C fragment made on the CSD (Cambridge Structural Database, ConQuest Version 1.18)[1] results in 6278 hits (organocobalt compounds) which include 654 Co–C≡N compounds. Limiting the search to only Co–*aromatic*, gave only 183 compounds, while just 17 compounds (less than 0.3% of the total number of organocobalt compounds) are obtained by further restricting to the Co–Ph fragment. It is thus evident that phenylcobalt compounds are rarely investigated. Another search combining any metal atom (other than cobalt) with Co–C fragment reveals that a large of number (2235 hits) of heterometallic compounds has been structurally reported, 63 of them being heterometallic Co-Sn systems including eight heterotrimetallic and one heterotetrametallic. However, no compound containing the Co(Ph)-Sn fragment has been found. In addition, a large number (2708) of phenyltin(IV) compounds is known but a search combining cobalt and phenyltin(IV) results only in 27 Co-Sn(Ph) compounds. No compound with Co–Ph and Sn–Ph fragments had been reported, and thus complex **1** appears to be the first example.

Another search for the alkoxido bridged transition metal-Sn systems resulted in only 34 results and only one (a Co^{III}-Sn^{IV} structure) with a methoxide bridge. Thus, compound **1** is the second one having a methoxido bridge between Co^{III} and Sn^{IV} ions.

A total of 94 hits were found by the search made for the heterometallic combination of Ni/Cu and Sn–C fragments. Excluding the C≡N moiety and restricting the search to Sn–Ph results in only 15 compounds leading us to conclude that **2** and **3** also belong to a rare family of compounds.

Concerning the involvement of the L^{2-} Schiff base, a search for this ligand in a transition metal organometallic compound (excluding the involvement of the C≡N moiety) resulted in 16 hits, with compounds of titanium(IV), cobalt(III) and rhodium(III).[1]

Moreover, intermetallic phenyl-group-shifts are not common,[2] the phenomenon being observed in some Grignard type compounds.[2a-d] In other cases the phenyl group shifted during an oxidative addition or insertion of other molecules in Sn–C bonds.[2e-g] Phenyl shifting was also reported for a Os-Sn system while reacted with CO.[2h] To our knowledge, the reaction leading to the heterometallic Schiff base system compound **1** has never been reported.

References:

1 F. H. Allen, *Acta Crystallogr*., 2002, **B58**, 380–388.

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Table S1. Crystallographic data for **1**–**3** and **1A**.

	1	**2**	**3**	**1A**
Formula	$C_{29}H_{27}Cl_2N_2O_3CoSn$	$C_{28}H_{24}Cl_2N_2O_2NiSn$	$C_{28}H_{24}Cl_2N_2O_2CuSn$	$C_{22}H_{21}N_2O_3Co$
FW	700.04	668.79	673.62	420.34
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic
Space group	*Pbca*	*P*21/*n*	*P*21/*n*	*Cc*
a/Å	16.5737(9)	11.1756(6)	11.2255(7)	18.206(2)
b/Å	17.3918(9)	15.6737(9)	15.7117(10)	14.7370(17)
c/Å	19.3984(10)	15.6480(8)	15.6670(9)	6.7877(8)
α/°	90.0	90.0	90.0	90
β/°	90.0	95.011(2)	94.998(2)	90.1230(10)
γ/°	90.0	90.0	90.0	90
V/Å^3	5591.5(5)	2730.5(3)	2752.7(3)	1821.2(4)
Z	8	4	4	4
T/K	298(2)	298(2)	298(2)	298(2)
θ/°	2.342 – 25.419	2.339 – 28.358	2.593 – 26.463	2.237 – 25.103
μ (Mo Kα)/mm^{-1}	1.712	1.828	1.902	0.969
ρ_{calcd}/g cm^{-3}	1.663	1.627	1.625	1.533
F(000)	2800	1336	1340	872
Index ranges	$-20\le h\le 20$	$-14\le h\le 14$	$-14\le h\le 14$	$-21\le h\le 21$
	$-20\le k\le 20$	$-20\le k\le 20$	$-19\le k\le 19$	$-17\le k\le 17$
	$-23\le l\le 23$	$-20\le k\le 20$	$-19\le l\le 19$	$-8\le l\le 8$
Rfs. collected	79912	71936	57538	18159
Rfs. unique/observed	5140/3393	6806/5805	5654/4690	3208/2616
R_{int}	0.1604	0.0293	0.0417	0.0844
R_1/ wR_2 [I > 2σ(I)]	0.0362/0.0563	0.0235/0.0519	0.0239/0.0511	0.0471/0.0846
R_1/ wR_2 [for all F_o^2]	0.0818/0.0664	0.0327/0.0572	0.0360/0.0558	0.0707/0.0920
GOF on F^2	1.045	1.048	1.027	1.098

Table S2. Calculated total energies, enthalpies, Gibbs free energies (in Hartree) and entropies (in cal/mol·K) (spin state is indicated in superscript).

	E_g 6-31G(d)	E_s 6-311+G(d,p)	H_g	H_s	S_g	S_s	G_g	G_s
^{1}**1**	-2525.151533	-2525.657252	-2524.616528	-2525.122247	223.16	149.47	-2524.722560	-2525.193265
^{3}**1**	-2525.117956							
^{5}**1**	-2525.097045							
^{2}**4**	-2525.754301	-2526.269386	-2525.207549	-2525.722634	239.51	160.59	-2525.321346	-2525.798934
^{4}**4**	-2525.752203	-2526.256379	-2525.206275	-2525.710451	242.21	162.42	-2525.321356	-2525.787624
^{2}**6**	-2525.710732	-2526.224968	-2525.164063	-2525.678299	240.59	161.32	-2525.278376	-2525.754948
^{4}**6**	-2525.678727		-2525.134344		251.40		-2525.253793	
^{1}**5**	-2525.120504	-2525.627399	-2524.585856	-2525.092751	230.61	154.54	-2524.695427	-2525.166176
^{3}**5**	-2525.120096	-2525.625356	-2524.586063	-2525.091323	237.93	159.51	-2524.699113	-2525.167113
^{1}**7**	-2525.100126	-2525.609229	-2524.566218	-2525.075321	224.67	150.50	-2524.672967	-2525.146827
^{3}**7**	-2525.077077		-2524.544873		232.27		-2524.655231	
^{2}**TS1**	-2525.702418	-2526.222456	-2525.157375	-2525.677413	233.76	156.68	-2525.268442	-2525.751855
^{4}**TS1**	-2525.678548	-2526.190007	-2525.135107	-2525.646566	243.90	163.57	-2525.250994	-2525.724285
^{1}**TS2**	-2525.095339	-2525.605733	-2524.562187	-2525.072581	218.31	146.17	-2524.665915	-2525.142032

Table S3. Cartesian atomic coordinates (Å) of the calculated structures.

^{1}1

C	-0.925829	2.459491	0.258592
C	-2.189494	2.729203	0.826001
H	-2.735744	1.903431	1.274058
C	-2.726399	4.008332	0.799842
H	-3.707647	4.180155	1.239269
C	-2.024643	5.077990	0.216632
H	-2.452345	6.077531	0.200943
C	-0.780490	4.836012	-0.336423
H	-0.216836	5.650960	-0.790719
C	-0.204013	3.542164	-0.330095
C	1.100404	3.398081	-0.918588
H	1.541521	4.307901	-1.343217
C	3.160603	2.306315	-1.511676
H	3.856921	2.453832	-0.675531
H	3.309142	3.114940	-2.240257
C	3.390447	0.931936	-2.147617
H	2.903740	0.894365	-3.132190
H	4.460540	0.723099	-2.285222
C	3.167454	-1.293691	-1.248366
H	4.052335	-1.551040	-1.843388

C	2.569133	-2.366734	-0.500902
C	3.249591	-3.609017	-0.478985
H	4.200780	-3.688370	-1.005469
C	2.733667	-4.703749	0.189822
H	3.269807	-5.649637	0.199246
C	1.499513	-4.574503	0.851589
H	1.075815	-5.428960	1.376837
C	0.804365	-3.373772	0.845686
H	-0.153100	-3.280682	1.350599
C	1.315970	-2.243488	0.175219
C	0.172570	-0.143845	-3.313476
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H	0.750630	-1.078040	-3.367945
H	-0.779664	-0.293559	-3.838260
C	2.208779	0.877946	1.329813
C	3.602320	0.768808	1.471309
H	4.231284	0.517017	0.620318
C	4.229075	0.957901	2.710486
H	5.312651	0.862060	2.782249
C	3.474227	1.259464	3.843639
H	3.958643	1.406665	4.807777
C	2.087032	1.364018	3.722504
H	1.477448	1.593503	4.596564
C	1.463103	1.176126	2.483716
H	0.382348	1.257030	2.423685
C	-2.518696	-1.115189	1.062178
C	-1.833132	-1.163931	2.284318
H	-0.767413	-0.951800	2.323116
C	-2.521302	-1.481567	3.460518
H	-1.983387	-1.515364	4.407175
C	-3.891624	-1.752559	3.422379
H	-4.424624	-2.000255	4.339284
C	-4.576901	-1.702807	2.206076
H	-5.645289	-1.911113	2.170823
C	-3.894587	-1.383560	1.027299
H	-4.442626	-1.335089	0.087970
N	1.797717	2.310343	-0.974331
N	2.756378	-0.066592	-1.276347
O	-0.458758	1.210121	0.310285
O	0.609823	-1.111391	0.186954
O	-0.060328	0.269956	-1.973562
Cl	-3.307526	0.517569	-1.969445
Cl	-1.511946	-2.774209	-1.996760
Co	1.255769	0.614889	-0.356571
Sn	-1.512419	-0.650473	-0.792756

^{3}1

C	-1.404188	2.336363	0.093084
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H	-3.240474	1.624910	0.944944
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C	-2.750787	4.835911	-0.119152
H	-3.269799	5.787974	-0.200658
C	-1.444615	4.708025	-0.552135
H	-0.929204	5.569470	-0.977397
C	-0.735052	3.482200	-0.459901
C	0.618614	3.508121	-0.961541
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C	2.854001	2.737514	-1.437765
H	3.504253	2.945205	-0.576549
H	2.915476	3.589016	-2.130667
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C	3.435854	-0.839895	-1.300632
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C	2.969550	-1.991987	-0.558970
C	3.808835	-3.134705	-0.599275
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C	1.437912	-3.277552	0.846118
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H	0.780780	0.588335	-3.754687
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C	1.953936	1.279681	1.455161
C	3.340225	1.292078	1.647484
H	4.019325	1.035043	0.838489
C	3.873781	1.609362	2.904381
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C	3.028334	1.922932	3.969170
H	3.443774	2.173129	4.944000
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H	0.973615	2.145854	4.600606
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H	0.026410	1.562617	2.392951
C	-2.310169	-1.484289	1.108285
C	-1.607865	-1.411341	2.319158
H	-0.583701	-1.047272	2.335926
C	-2.225265	-1.810110	3.509417
H	-1.675115	-1.750927	4.447833
C	-3.540566	-2.282046	3.496441
H	-4.018218	-2.592429	4.424726
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H	-5.267412	-2.720160	2.274839
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H	-4.191674	-2.008298	0.165337
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O	-0.820210	1.150679	0.235674
O	0.858082	-1.070062	0.303411
O	-0.031175	0.153632	-1.923582
Cl	-3.339666	-0.049985	-2.012241
Cl	-1.081574	-3.015208	-1.906196
Co	1.160648	0.749307	-0.276405
Sn	-1.424449	-0.877562	-0.765949

^{5}1

C	-1.108385	2.459183	-0.048010
C	-2.344951	2.695246	0.594409
H	-2.770090	1.892516	1.190052
C	-3.004345	3.907282	0.455124
H	-3.958277	4.052614	0.959380
C	-2.465478	4.941963	-0.331385
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C	0.703378	3.404968	-1.542316
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H	3.613051	2.605891	-1.529574
H	2.789174	3.135110	-3.021445
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H	2.211966	0.832192	-3.598076
H	3.943220	0.799799	-3.168788
C	3.034811	-1.198467	-1.762059
H	3.772794	-1.457145	-2.535758
C	2.646536	-2.274110	-0.886370
C	3.391166	-3.476953	-0.959406

H	4.237348	-3.521471	-1.645269
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C	1.959285	-4.497630	0.678272
H	1.685555	-5.358650	1.285769
C	1.197542	-3.341170	0.762460
H	0.332384	-3.286714	1.417288
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C	-0.976262	-0.552164	-3.467935
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H	-0.985797	-1.634556	-3.667232
H	-1.981056	-0.150984	-3.665783
C	2.385587	1.234968	1.411807
C	3.572651	0.552365	1.721179
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C	4.337417	0.933252	2.830090
H	5.258314	0.399315	3.063001
C	3.915508	1.991677	3.640586
H	4.508195	2.284282	4.506124
C	2.727379	2.667415	3.345683
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C	-1.163661	-0.937158	2.561545
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C	-3.828999	-1.504550	3.187472
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N	2.586506	0.014985	-1.719428
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O	0.761483	-1.111046	0.103522
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Cl	-3.736445	-0.032550	-1.370538
Cl	-1.737841	-3.265668	-1.283364
Co	1.333078	0.757587	-0.264641
Sn	-1.587533	-0.930827	-0.568216

^{2}4

Sn	-0.876183	-1.150282	1.116144
Co	0.923403	1.219088	-0.714833
Cl	-3.049080	-0.847271	2.258840
Cl	0.199375	-2.977185	2.340434
O	1.199875	-0.671127	-0.403920
O	-0.955678	0.830672	-0.779087
C	-1.665770	-2.261237	-0.577841
C	0.078270	0.517434	2.136712
C	-2.871371	-2.958116	-0.407802
H	-3.406141	-2.905445	0.537619
C	-3.406565	-3.713134	-1.457769
H	-4.343959	-4.247911	-1.310833
C	-2.744959	-3.783167	-2.685072
H	-3.162966	-4.371537	-3.500681
C	-1.540656	-3.096674	-2.859032
H	-1.013775	-3.152122	-3.811470
C	-1.004146	-2.341288	-1.811363
H	-0.062636	-1.817702	-1.947533
C	2.361785	-1.310075	-0.461168
C	2.372820	-2.726975	-0.480939
H	1.422360	-3.249335	-0.433774
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H	3.526511	-4.524866	-0.551174
C	4.805651	-2.777439	-0.576437
H	5.732550	-3.344553	-0.617463
C	4.824201	-1.396141	-0.549017
H	5.774131	-0.860981	-0.566975
C	3.627992	-0.636792	-0.498422
C	3.749459	0.792651	-0.442915
H	4.764754	1.193039	-0.328939
N	2.765284	1.635079	-0.503225
C	2.999575	3.070265	-0.306464
H	2.860503	3.297219	0.760760
H	4.020306	3.359367	-0.595278
C	1.946083	3.807209	-1.131300
H	2.220244	3.772302	-2.196401
H	1.859334	4.860839	-0.830353
N	0.680444	3.085923	-0.954297
C	-0.449080	3.716347	-1.056441
H	-0.418723	4.803990	-1.197397
C	-1.750935	3.115540	-1.022276
C	-1.948790	1.701395	-0.897393
C	-3.281111	1.218954	-0.909656
H	-3.437206	0.147921	-0.816094

C	-4.356411	2.085040	-1.025868
H	-5.366025	1.677089	-1.024454
C	-4.165090	3.475824	-1.143090
H	-5.016764	4.145801	-1.234066
C	-2.875609	3.971150	-1.142880
H	-2.700671	5.043204	-1.238392
C	-0.638125	1.693758	2.409857
H	-1.668755	1.798878	2.078173
C	-0.045356	2.733545	3.134691
H	-0.616816	3.636692	3.345703
C	1.263393	2.604064	3.608361
H	1.717638	3.406842	4.188065
C	1.976064	1.427232	3.359074
H	2.986310	1.306276	3.748957
C	1.386349	0.388418	2.629921
H	1.947436	-0.529182	2.465216
O	0.728394	0.854864	-3.008271
H	-0.116884	0.405402	-2.812229
C	1.552766	-0.007593	-3.801693
H	1.772284	-0.952185	-3.286763
H	2.490998	0.527955	-3.974723
H	1.081803	-0.216465	-4.772451

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Sn	-0.133961	-1.991066	-0.351568
Co	0.156449	1.653189	0.323552
Cl	1.591428	-3.588949	-1.011554
Cl	-2.110465	-3.425941	-0.183072
O	-1.445043	0.463701	0.452185
O	1.561123	0.363086	-0.265635
C	0.315938	-1.847508	1.767129
C	-0.547638	-1.021171	-2.233006
C	1.624290	-1.613905	2.222646
H	2.438710	-1.467428	1.517744
C	1.900798	-1.577585	3.596554
H	2.920646	-1.399170	3.934794
C	0.877561	-1.789722	4.526435
H	1.095574	-1.771465	5.593164
C	-0.420630	-2.044134	4.077411
H	-1.220604	-2.226629	4.793617
C	-0.700484	-2.072040	2.706243
H	-1.713465	-2.286738	2.374787
C	-2.719438	0.790518	0.401647
C	-3.702080	-0.210229	0.638144
H	-3.359601	-1.223360	0.827619

C	-5.056569	0.072652	0.602458
H	-5.769106	-0.731110	0.784023
C	-5.524329	1.374341	0.333071
H	-6.590305	1.587710	0.306450
C	-4.598000	2.370515	0.100322
H	-4.933229	3.386126	-0.113456
C	-3.199897	2.121851	0.126260
C	-2.348335	3.247357	-0.130782
H	-2.871644	4.189545	-0.353509
N	-1.049764	3.258562	-0.117337
C	-0.336578	4.497162	-0.432600
H	-0.112214	4.512470	-1.510249
H	-0.936990	5.389186	-0.196334
C	0.985079	4.496114	0.348852
H	0.772291	4.652160	1.417951
H	1.645663	5.309257	0.008124
N	1.583228	3.181245	0.178980
C	2.843438	3.053615	-0.063739
H	3.470285	3.958331	-0.105710
C	3.527738	1.810229	-0.314517
C	2.863960	0.537900	-0.425330
C	3.675576	-0.581694	-0.745159
H	3.192556	-1.549167	-0.854342
C	5.047528	-0.467494	-0.919565
H	5.624307	-1.360418	-1.157442
C	5.694676	0.774099	-0.800229
H	6.769651	0.859247	-0.940906
C	4.928038	1.888381	-0.509718
H	5.402116	2.867005	-0.424851
C	0.498554	-0.619437	-3.075032
H	1.534858	-0.752313	-2.775284
C	0.215632	-0.045627	-4.318608
H	1.034481	0.258014	-4.969507
C	-1.109095	0.129380	-4.727714
H	-1.326781	0.573356	-5.698173
C	-2.152757	-0.279477	-3.894076
H	-3.187449	-0.157717	-4.211468
C	-1.875401	-0.858272	-2.651130
H	-2.698515	-1.186658	-2.020849
O	0.623945	1.533399	2.463118
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C	-0.440738	1.685739	3.421839
H	-1.257644	0.983726	3.221065
H	-0.803870	2.713050	3.326314
H	-0.055321	1.531105	4.437093

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Sn	0.995899	-1.094892	1.076055
Co	-1.095390	1.079838	-0.791372
Cl	0.384619	-3.286810	2.000701
Cl	2.879488	-0.321022	2.452561
O	0.776400	1.069390	-0.478950
O	-0.989127	-0.822729	-0.731834
C	2.156960	-1.794747	-0.614935
C	-0.534476	0.054273	2.114772
C	3.405473	-2.372345	-0.336016
H	3.773675	-2.426916	0.686425
C	4.199087	-2.870547	-1.374662
H	5.166798	-3.314976	-1.146038
C	3.753325	-2.799469	-2.696397
H	4.372158	-3.188163	-3.504034
C	2.510153	-2.227899	-2.977321
H	2.154981	-2.169174	-4.005601
C	1.712319	-1.727143	-1.942478
H	0.747559	-1.284171	-2.171251
C	1.600135	2.103108	-0.526947
C	2.995509	1.871203	-0.591219
H	3.344166	0.843116	-0.613988
C	3.889289	2.929346	-0.616121
H	4.956284	2.717900	-0.663781
C	3.445574	4.267014	-0.579280
H	4.160804	5.085776	-0.598181
C	2.089331	4.519200	-0.514054
H	1.721218	5.544770	-0.480207
C	1.145733	3.461158	-0.491753
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H	-0.489850	4.844750	-0.224271
N	-1.226703	2.943773	-0.450872
C	-2.607421	3.383818	-0.208809
H	-2.815788	3.283043	0.866354
H	-2.748134	4.434736	-0.496782
C	-3.516466	2.452700	-1.003970
H	-3.458410	2.700567	-2.072915
H	-4.561660	2.526794	-0.673255
N	-2.992333	1.094989	-0.834613
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H	-4.842597	0.250057	-1.083122
C	-3.345687	-1.299685	-1.046107
C	-1.969401	-1.684530	-0.943924
C	-1.660398	-3.063440	-1.044088
H	-0.620804	-3.365660	-0.960892

C	-2.658102	-4.006643	-1.228247
H	-2.383274	-5.057945	-1.296826
C	-4.012909	-3.631149	-1.326257
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C	-4.340280	-2.292701	-1.235274
H	-5.380311	-1.975066	-1.312417
C	-1.766834	-0.537619	2.437572
H	-1.979616	-1.559324	2.130316
C	-2.720821	0.168234	3.177674
H	-3.668415	-0.306932	3.428465
C	-2.450867	1.468673	3.614852
H	-3.187946	2.010904	4.205985
C	-1.219374	2.058624	3.315210
H	-0.988821	3.059183	3.679908
C	-0.264079	1.353824	2.573351
H	0.702143	1.813845	2.377172
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C	-0.015019	1.616557	-3.312795
H	0.816485	0.902021	-3.205212
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H	-0.298887	1.648748	-4.378860

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Sn	1.291775	-0.898307	1.088993
Co	-1.334627	0.868581	-0.951155
Cl	0.946949	-3.016582	2.263247
Cl	3.293734	0.092305	2.115981
O	0.535541	1.090495	-0.784986
O	-1.050787	-0.984984	-0.470105
C	2.258404	-1.636769	-0.706008
C	-0.135847	0.296135	2.202205
C	3.616329	-1.978276	-0.605019
H	4.158392	-1.819900	0.324466
C	4.292212	-2.510942	-1.707906
H	5.346052	-2.770504	-1.617237
C	3.621091	-2.709340	-2.916319
H	4.148907	-3.124217	-3.773928
C	2.269397	-2.373225	-3.018920
H	1.738033	-2.523965	-3.957991
C	1.588037	-1.840333	-1.919686
H	0.539556	-1.577811	-2.013077
C	1.191294	2.234779	-0.870033
C	2.587684	2.191149	-1.107789
H	3.052190	1.216239	-1.228174
C	3.335157	3.355305	-1.175335

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C	0.581770	3.519824	-0.692003
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H	-3.235619	2.696315	1.033457
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C	-3.897045	1.995817	-0.909067
H	-3.862665	2.337461	-1.952532
H	-4.944285	1.932150	-0.582685
N	-3.234061	0.693149	-0.839298
C	-3.905585	-0.410329	-0.768394
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C	-1.946295	-1.960900	-0.536374
C	-1.510872	-3.303500	-0.425009
H	-0.450502	-3.493545	-0.291193
C	-2.413066	-4.355369	-0.477108
H	-2.038527	-5.374284	-0.392858
C	-3.794047	-4.129154	-0.629876
H	-4.491017	-4.962906	-0.665719
C	-4.246514	-2.827080	-0.727737
H	-5.311506	-2.623314	-0.840419
C	-1.352930	-0.261271	2.621028
H	-1.607851	-1.285770	2.358676
C	-2.239797	0.485708	3.404216
H	-3.175099	0.036691	3.736766
C	-1.916347	1.793448	3.779244
H	-2.600648	2.369056	4.401575
C	-0.697060	2.347158	3.378294
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C	0.193027	1.600334	2.598419
H	1.151260	2.033892	2.320686
O	-1.502038	1.028344	-2.795343
C	-0.465221	0.781731	-3.711100
H	0.534415	0.815021	-3.253933
H	-0.506416	1.532136	-4.519156
H	-0.592367	-0.211384	-4.177646

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Sn	-1.796897	-0.824317	-0.688357

Co	1.569297	0.344514	-0.252229
Cl	-2.960948	-3.002807	-1.185348
Cl	-2.235249	0.489096	-2.827237
O	0.618573	-1.248368	0.267771
O	-0.131864	1.218833	-0.262635
C	-3.032245	-0.197902	1.031911
C	1.957059	0.845271	1.577630
C	-4.375247	-0.596658	1.108279
H	-4.826318	-1.176129	0.304454
C	-5.140225	-0.264968	2.231473
H	-6.184838	-0.569536	2.282300
C	-4.564918	0.446946	3.287746
H	-5.161247	0.697849	4.164003
C	-3.222689	0.829660	3.222651
H	-2.768356	1.376316	4.048106
C	-2.455084	0.510197	2.096985
H	-1.411616	0.818490	2.054579
C	1.103810	-2.475325	0.368882
C	0.248407	-3.523890	0.790123
H	-0.784777	-3.287724	1.029510
C	0.700317	-4.830413	0.876635
H	0.005697	-5.607894	1.190043
C	2.033925	-5.165308	0.569908
H	2.377415	-6.194133	0.644603
C	2.896725	-4.159730	0.180863
H	3.938224	-4.388248	-0.046794
C	2.466329	-2.812553	0.072629
C	3.444912	-1.826890	-0.282484
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N	3.231241	-0.554510	-0.405998
C	4.344881	0.371838	-0.623633
H	4.646026	0.775103	0.353381
H	5.208074	-0.133545	-1.078559
C	3.815798	1.494239	-1.509689
H	3.733070	1.139195	-2.546779
H	4.476734	2.371758	-1.491266
N	2.469261	1.827516	-1.028562
C	1.954790	2.981376	-1.316216
H	2.596209	3.713414	-1.821897
C	0.612537	3.395076	-1.037744
C	-0.374620	2.497053	-0.513752
C	-1.670197	3.019306	-0.278296
H	-2.428226	2.354763	0.122733
C	-1.973832	4.341445	-0.556706
H	-2.984089	4.700865	-0.366954

C	-1.007180	5.221975	-1.081247
H	-1.260390	6.256720	-1.299038
C	0.265563	4.742406	-1.315746
H	1.034320	5.400356	-1.721577
C	1.818830	2.169984	2.013897
H	1.499524	2.952575	1.331776
C	2.075078	2.518031	3.346583
H	1.954702	3.555271	3.658850
C	2.477097	1.548977	4.266821
H	2.676821	1.819993	5.302401
C	2.615572	0.226458	3.842024
H	2.920862	-0.547176	4.546318
C	2.357516	-0.122767	2.510618
H	2.464739	-1.165049	2.222682
O	1.111934	-0.099555	-2.532880
H	0.226912	0.295143	-2.694271
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H	0.410578	-2.069359	-2.795970
H	2.154909	-1.778557	-3.046301
H	0.978365	-1.242266	-4.278307

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Sn	-1.545942	-1.336567	-0.634736
Co	1.373561	0.671525	-0.194226
Cl	-2.081284	-3.759903	-0.915638
Cl	-2.233139	-0.433358	-2.895200
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O	-0.475404	1.202985	-0.491919
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C	1.497358	1.369953	1.660411
C	-4.154793	-1.609162	1.109009
H	-4.381336	-2.407506	0.404353
C	-5.038231	-1.346478	2.161371
H	-5.953846	-1.929011	2.255089
C	-4.744117	-0.346960	3.092920
H	-5.430841	-0.149768	3.914972
C	-3.565375	0.393647	2.973995
H	-3.328432	1.167175	3.703429
C	-2.682282	0.143129	1.917763
H	-1.768317	0.728261	1.832392
C	1.836364	-2.242792	0.407425
C	1.356265	-3.540017	0.731647
H	0.287446	-3.664063	0.884080
C	2.206596	-4.627819	0.821575
H	1.790361	-5.605817	1.058437

C	3.593994	-4.488349	0.615549
H	4.255441	-5.347769	0.694575
C	4.095355	-3.238231	0.314715
H	5.166580	-3.104716	0.159664
C	3.256910	-2.097718	0.194706
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H	5.014354	-0.905300	-0.152198
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C	4.151278	1.507981	-0.477114
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C	3.407098	2.428344	-1.455978
H	3.474948	2.002288	-2.467914
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H	1.694959	4.335487	-1.884656
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C	-0.979371	2.405124	-0.745724
C	-2.375388	2.606971	-0.621632
H	-2.985497	1.768660	-0.300595
C	-2.959168	3.830898	-0.909413
H	-4.037485	3.940617	-0.804225
C	-2.183532	4.922139	-1.339312
H	-2.648983	5.878000	-1.567981
C	-0.817727	4.752254	-1.475800
H	-0.197223	5.581450	-1.816911
C	1.045801	2.647088	1.994963
H	0.616386	3.308338	1.248062
C	1.128843	3.086200	3.323772
H	0.767969	4.082443	3.577731
C	1.665090	2.257495	4.310919
H	1.729341	2.602603	5.341548
C	2.114033	0.980780	3.967483
H	2.527961	0.319878	4.728341
C	2.029507	0.529442	2.643456
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O	1.190451	0.027715	-2.438288
H	0.243932	0.176934	-2.648156
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H	1.021499	-2.063132	-2.639526
H	2.650302	-1.350667	-2.796256
H	1.470042	-1.171159	-4.126487

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Sn	1.310033	-0.135583	1.102001
Co	-1.379652	0.199581	-0.633403
Cl	1.055448	-1.879528	2.742872
Cl	1.822903	1.532710	2.787950
O	0.032046	1.311596	0.114329
O	-0.159218	-1.221385	-0.148612
C	3.008028	-0.352531	-0.181586
C	-2.219143	0.073871	1.168794
C	4.297314	-0.504415	0.350167
H	4.460017	-0.515552	1.427253
C	5.390163	-0.639925	-0.511200
H	6.391284	-0.760508	-0.100210
C	5.195272	-0.617303	-1.895088
H	6.048282	-0.720956	-2.564366
C	3.910158	-0.459072	-2.421223
H	3.761504	-0.436962	-3.499883
C	2.806272	-0.327331	-1.571523
H	1.802849	-0.195879	-1.987041
C	0.294242	2.548955	-0.365759
C	1.575094	3.114236	-0.268479
H	2.385868	2.534957	0.158670
C	1.819433	4.415748	-0.697846
H	2.825932	4.819154	-0.602413
C	0.796369	5.202694	-1.239841
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C	-0.471133	4.653273	-1.355337
H	-1.281839	5.240759	-1.785777
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H	-3.663379	-0.016541	-3.041824
H	-4.760523	-0.708851	-1.817572
N	-2.674120	-0.891290	-1.421306
C	-2.527623	-2.153502	-1.642528
H	-3.334037	-2.677829	-2.168643
C	-1.380725	-2.962388	-1.290917
C	-0.225843	-2.484330	-0.595060
C	0.841329	-3.377906	-0.385583
H	1.730371	-3.029991	0.128477

C	0.771715	-4.696707	-0.818570
H	1.618672	-5.355499	-0.634810
C	-0.363930	-5.181781	-1.481870
H	-0.414889	-6.215069	-1.816215
C	-1.417586	-4.312980	-1.710118
H	-2.305535	-4.662863	-2.236332
C	-2.731372	-1.135356	1.672314
H	-2.672659	-2.046454	1.078242
C	-3.303251	-1.217020	2.946957
H	-3.680070	-2.173855	3.308629
C	-3.379167	-0.082456	3.758261
H	-3.819086	-0.144514	4.752642
C	-2.869879	1.128077	3.285051
H	-2.904572	2.019208	3.911742
C	-2.299171	1.201174	2.007879
H	-1.895914	2.158066	1.678096
O	-0.358357	0.322212	-2.307519
C	-0.906568	0.461404	-3.571455
H	-1.568378	1.351103	-3.682984
H	-1.498091	-0.420378	-3.911651
H	-0.101681	0.589064	-4.320066

^{3}7

Sn	1.421611	0.312112	1.015746
Co	-1.379676	-0.108233	-0.618260
Cl	1.114984	-1.068234	2.950622
Cl	2.276151	2.151333	2.400782
O	-0.190594	1.433752	0.223100
O	0.094826	-1.252045	-0.007013
C	3.065362	0.001264	-0.327583
C	-2.277345	-0.293350	1.180161
C	4.375924	0.147651	0.150351
H	4.562826	0.436983	1.183244
C	5.454570	-0.067693	-0.712702
H	6.472588	0.039161	-0.341421
C	5.224713	-0.411787	-2.047472
H	6.066716	-0.575083	-2.718673
C	3.917028	-0.539263	-2.523752
H	3.739242	-0.795551	-3.567244
C	2.829045	-0.338896	-1.667725
H	1.808502	-0.419117	-2.042366
C	-0.271802	2.653808	-0.366227
C	0.825604	3.529741	-0.371526
H	1.759467	3.203680	0.072133
C	0.731260	4.819201	-0.885061

H	1.608978	5.462421	-0.855207
C	-0.471735	5.290907	-1.419856
H	-0.553531	6.303044	-1.808643
C	-1.558102	4.431845	-1.453816
H	-2.496686	4.772766	-1.890338
C	-1.499952	3.103439	-0.967805
C	-2.713959	2.331245	-1.220020
H	-3.566547	2.918253	-1.589813
N	-2.850599	1.057757	-1.105384
C	-4.073461	0.320615	-1.406795
H	-4.577791	0.120401	-0.452454
H	-4.753061	0.898127	-2.050962
C	-3.701295	-1.028110	-2.079955
H	-3.501411	-0.854656	-3.146847
H	-4.543446	-1.731634	-2.002212
N	-2.487018	-1.547093	-1.459605
C	-2.053220	-2.750098	-1.595629
H	-2.655245	-3.481818	-2.156270
C	-0.797667	-3.270785	-1.066164
C	0.206508	-2.547713	-0.322635
C	1.357337	-3.255063	0.087485
H	2.112396	-2.720913	0.654638
C	1.537011	-4.599119	-0.205649
H	2.443286	-5.097848	0.134040
C	0.568505	-5.311959	-0.926647
H	0.706399	-6.365713	-1.156654
C	-0.569916	-4.642956	-1.339722
H	-1.333266	-5.180639	-1.902331
C	-2.620066	-1.558166	1.679401
H	-2.402628	-2.458543	1.109322
C	-3.220660	-1.695265	2.937033
H	-3.464868	-2.690625	3.308094
C	-3.494537	-0.569242	3.715590
H	-3.959169	-0.676620	4.694606
C	-3.156166	0.694799	3.229464
H	-3.352352	1.583764	3.828674
C	-2.554851	0.830834	1.971774
H	-2.293102	1.828112	1.625087
O	-0.400338	0.245190	-2.183085
C	-0.882205	0.297859	-3.488502
H	-1.711814	1.022303	-3.616947
H	-1.242720	-0.684968	-3.854166
H	-0.074762	0.616454	-4.170595

^{2}TS1

Sn	-0.970015	-0.938962	1.054105
Co	1.039875	1.018662	-0.591231
Cl	-2.847331	-0.012481	2.410049
Cl	0.028361	-2.672472	2.519106
O	1.044692	-0.910716	-0.548171
O	-0.853759	0.911249	-0.915794
C	-2.155553	-2.150802	-0.358312
C	0.843263	1.154921	1.407407
C	-3.418758	-2.621650	0.029927
H	-3.818541	-2.374518	1.012061
C	-4.180183	-3.403684	-0.846336
H	-5.158460	-3.767128	-0.533633
C	-3.689764	-3.717758	-2.116291
H	-4.283793	-4.326739	-2.796507
C	-2.435098	-3.246510	-2.511677
H	-2.048838	-3.487502	-3.501954
C	-1.672551	-2.465320	-1.636176
H	-0.696532	-2.100024	-1.950376
C	2.099194	-1.711523	-0.606164
C	1.896012	-3.113568	-0.632213
H	0.877486	-3.485097	-0.566886
C	2.964967	-3.989762	-0.726766
H	2.769589	-5.060876	-0.741174
C	4.291813	-3.521106	-0.795594
H	5.122275	-4.219397	-0.865977
C	4.517410	-2.158832	-0.758380
H	5.535667	-1.770774	-0.797256
C	3.448715	-1.231587	-0.662207
C	3.779883	0.163141	-0.583092
H	4.848839	0.409731	-0.564603
N	2.932945	1.139850	-0.500075
C	3.383038	2.515126	-0.283416
H	3.283565	2.735955	0.788771
H	4.434019	2.650119	-0.575675
C	2.452826	3.417814	-1.089860
H	2.715164	3.359330	-2.156564
H	2.529558	4.466446	-0.770858
N	1.087215	2.902577	-0.919481
C	0.076707	3.677213	-1.157974
H	0.281226	4.732014	-1.380332
C	-1.303591	3.282570	-1.173940
C	-1.711147	1.915509	-1.052008
C	-3.095019	1.625644	-1.114986
H	-3.405088	0.588639	-1.016642

C	-4.026995	2.636866	-1.286390
H	-5.084595	2.380457	-1.323348
C	-3.630869	3.983184	-1.409812
H	-4.372447	4.766936	-1.544332
C	-2.284376	4.289598	-1.356672
H	-1.952661	5.323582	-1.454575
C	0.068951	2.201321	1.955272
H	-0.717597	2.666761	1.367083
C	0.270717	2.634646	3.267125
H	-0.351367	3.434272	3.667176
C	1.245182	2.033196	4.069790
H	1.393673	2.365533	5.095738
C	2.008288	0.981781	3.550958
H	2.748617	0.482153	4.174515
C	1.810897	0.545581	2.239618
H	2.393673	-0.297378	1.875704
O	0.958177	0.834186	-2.926256
H	0.029230	0.584311	-2.744027
C	1.565755	-0.172887	-3.744735
H	1.478525	-1.169907	-3.295582
H	2.624853	0.086798	-3.833685
H	1.118257	-0.178696	-4.748608

^{4}TS1

Sn	-0.255083	1.600708	1.070740
Co	0.186103	-1.404851	-0.531566
Cl	1.666562	2.650540	2.254523
Cl	-2.141531	2.032082	2.598147
O	-1.502865	-0.361203	-0.191723
O	1.443837	0.068917	-0.895243
C	-0.543553	3.034769	-0.579238
C	0.584076	-1.646501	1.421025
C	0.311855	4.141559	-0.681569
H	1.095524	4.298771	0.057952
C	0.153628	5.059921	-1.725864
H	0.819191	5.919693	-1.793351
C	-0.855990	4.879740	-2.674194
H	-0.978538	5.596259	-3.485189
C	-1.712429	3.779993	-2.575732
H	-2.507604	3.639428	-3.307377
C	-1.555182	2.858932	-1.534133
H	-2.235780	2.012216	-1.469100
C	-2.753861	-0.776140	-0.290602
C	-3.814213	0.143402	-0.075251
H	-3.559555	1.154701	0.228141

C	-5.140417	-0.232324	-0.211209
H	-5.919308	0.509239	-0.039518
C	-5.493379	-1.551708	-0.552523
H	-6.537098	-1.838580	-0.655852
C	-4.485347	-2.479440	-0.728274
H	-4.734109	-3.514115	-0.966699
C	-3.113945	-2.136545	-0.602643
C	-2.172164	-3.219974	-0.734710
H	-2.620150	-4.218099	-0.855071
N	-0.882846	-3.131730	-0.685950
C	-0.046173	-4.326141	-0.687697
H	0.251516	-4.530817	0.351147
H	-0.584899	-5.205421	-1.073218
C	1.205823	-4.039471	-1.526957
H	0.924218	-4.018266	-2.590592
H	1.960372	-4.829621	-1.388425
N	1.714998	-2.720516	-1.165786
C	2.959491	-2.430730	-1.339228
H	3.651804	-3.222155	-1.667287
C	3.546338	-1.122252	-1.160479
C	2.769521	0.066583	-0.940544
C	3.463558	1.294105	-0.815729
H	2.878176	2.191616	-0.637756
C	4.846236	1.352037	-0.904098
H	5.344708	2.314027	-0.794960
C	5.608745	0.191616	-1.130090
H	6.692419	0.246689	-1.202695
C	4.954615	-1.021079	-1.259375
H	5.525452	-1.932532	-1.439744
C	1.886415	-1.566249	1.917512
H	2.713660	-1.257165	1.285759
C	2.133506	-1.871751	3.262252
H	3.150553	-1.798398	3.644884
C	1.087210	-2.249150	4.106440
H	1.283228	-2.477189	5.152653
C	-0.215037	-2.312426	3.606121
H	-1.043522	-2.584145	4.258903
C	-0.474813	-2.005458	2.264303
H	-1.498050	-2.036896	1.900765
O	-0.075507	-1.015593	-2.775182
H	0.500108	-0.234010	-2.638172
C	-1.266018	-0.622585	-3.471035
H	-1.753601	0.230750	-2.986366
H	-1.942247	-1.481584	-3.453594
H	-1.032386	-0.371016	-4.514873

TS2

Sn	-0.670972	0.978588	0.913539
Co	0.851745	-1.105684	-0.715021
Cl	0.632070	2.345606	2.444299
Cl	-2.286064	0.158118	2.542362
O	-1.026660	-0.760376	-0.461799
O	0.971591	0.831117	-0.580201
C	-1.848466	2.369353	-0.234391
C	1.061471	-1.207366	1.312138
C	-2.849566	3.124714	0.394304
H	-3.038315	3.011727	1.460941
C	-3.620569	4.024542	-0.348681
H	-4.394427	4.609868	0.145932
C	-3.398932	4.170656	-1.720641
H	-4.001171	4.870762	-2.297975
C	-2.405895	3.416791	-2.351620
H	-2.233399	3.525664	-3.421488
C	-1.629933	2.517079	-1.612830
H	-0.858949	1.933044	-2.112729
C	-2.034100	-1.633570	-0.613582
C	-3.362880	-1.175206	-0.569783
H	-3.542797	-0.117795	-0.399549
C	-4.424282	-2.056305	-0.741756
H	-5.442002	-1.672143	-0.699871
C	-4.200472	-3.422330	-0.970642
H	-5.035314	-4.105845	-1.105219
C	-2.895622	-3.886112	-1.025005
H	-2.699613	-4.942526	-1.208233
C	-1.792805	-3.019427	-0.852989
C	-0.469728	-3.605316	-0.922744
H	-0.432225	-4.694280	-1.045941
N	0.647769	-2.970029	-0.831905
C	1.938764	-3.661379	-0.799446
H	2.211767	-3.806597	0.254969
H	1.881702	-4.643521	-1.288494
C	2.958497	-2.751944	-1.486129
H	2.803024	-2.782441	-2.571651
H	3.988948	-3.053386	-1.252158
N	2.687382	-1.374834	-1.055653
C	3.552699	-0.440434	-1.242038
H	4.557142	-0.732358	-1.572458
C	3.333483	0.982473	-1.091127
C	2.070461	1.573665	-0.787347
C	1.978047	2.976567	-0.735192
H	1.013769	3.427213	-0.520542

C	3.094272	3.775248	-0.954056
H	2.987934	4.857428	-0.902058
C	4.343096	3.206055	-1.242935
H	5.213182	3.834846	-1.415681
C	4.445897	1.826098	-1.314345
H	5.403247	1.363786	-1.554366
C	2.209463	-0.681286	1.953007
H	2.849137	0.022839	1.425159
C	2.551795	-1.024041	3.261879
H	3.439763	-0.591701	3.721490
C	1.746076	-1.907659	3.986849
H	2.006477	-2.171893	5.010896
C	0.592483	-2.430711	3.397253
H	-0.057308	-3.098161	3.961900
C	0.261166	-2.082060	2.085717
H	-0.654376	-2.492031	1.663786
O	0.830725	-0.982184	-2.657609
C	-0.339927	-1.135958	-3.391792
H	-1.153627	-0.446294	-3.091142
H	-0.757460	-2.165716	-3.356268
H	-0.124024	-0.926972	-4.456553

Table S4. Time variation in aerobic Baeyer–Villiger oxidation of cyclohexanone with the precatalyst **1**.[a]

Entry	Time (h)	Conversion[b] (%)	Yield[c] (%)	Selectivity[d] (%)	TON[e]	TOF[f] (h^{-1})
1	0.1	52	45.3	87.1	227	2265
2	0.25	71.6	62	86.6	310	1240
3	0.5	77.9	68.7	88.4	344	689
4	1	84.1	70.5	83.8	352	352
5	2	88.4	73.7	83.3	368	184
7	6	94.4	80.2	85.0	401	67
8	10	95.2	79.8	83.8	399	40

[a]Reaction conditions: cyclohexanone, 1 mmol; benzaldehyde, 2 mmol; dioxygen, 1 atm; precatalyst, 0.2 mol% (relative to cyclohexanone substrate); 1,2-DCE, 1.0 mL; reaction temperature, 50 ˚C (yield and TON determined by GC analysis). [b]Conversion of cyclohexanone. [c]Molar yield (%) based on the cyclohexanone, *i.e.* moles of ε-caprolactone per 100 mol of cyclohexanone. [d]Selectivity based on ε-caprolactone per 100 mol of converted cyclohexanone. [e]Turnover number (moles of ε-caprolactone per mole of **1**). [f]TON per reaction time.

Table S5. Aerobic Baeyer–Villiger oxidation of cyclohexanone catalyzed by **1**, using different heating/irradiation methods.[a]

Entry	Method	Conversion[b] (%)	Yield[c] (%)	Selectivity[d] (%)	TON[e]	TOF[f] (h^{-1})
1	Trad heat	84.1	70.5	83.8	352	352
2	MW	84.3	70.3	83.3	351	351
3	US	83.9	67.8	80.8	339	339

[a]Reaction conditions: cyclohexanone, 1 mmol; benzaldehyde, 2 mmol; dioxygen, 1 atm; precatalyst, 0.2 mol% (relative to cyclohexanone substrate); 1,2-DCE, 1.0 mL; reaction temperature, 50 ˚C; reaction time, 1 h (yield and TON determined by GC analysis); Trad heat = traditional heating; MW = microwave heating; US = ultrasound heating. [b]Conversion of cyclohexanone. [c]Molar yield (%) based on the cyclohexanone, *i.e.* moles of ε-caprolactone per 100 mol of cyclohexanone. [d]Selectivity based on ε-caprolactone per 100 mol of converted cyclohexanone. [e]Turnover number (moles of ε-caprolactone per mole of **1**). [f]TON per reaction time.