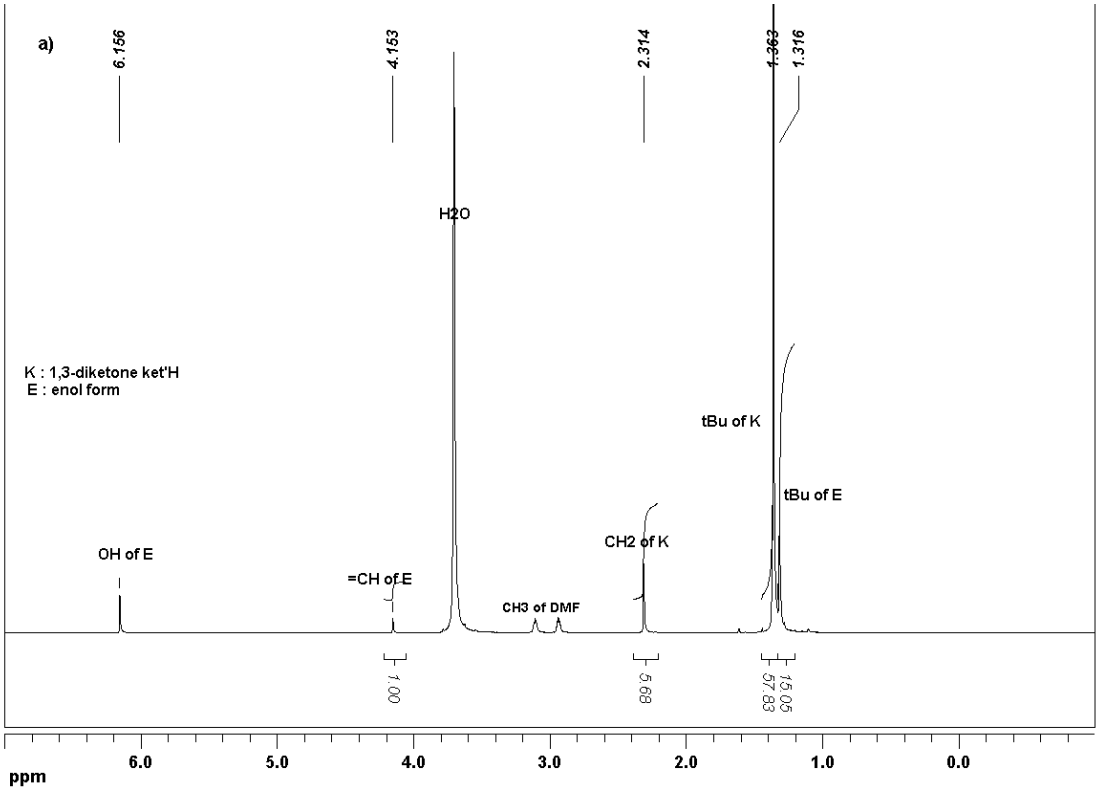
Supporting Information

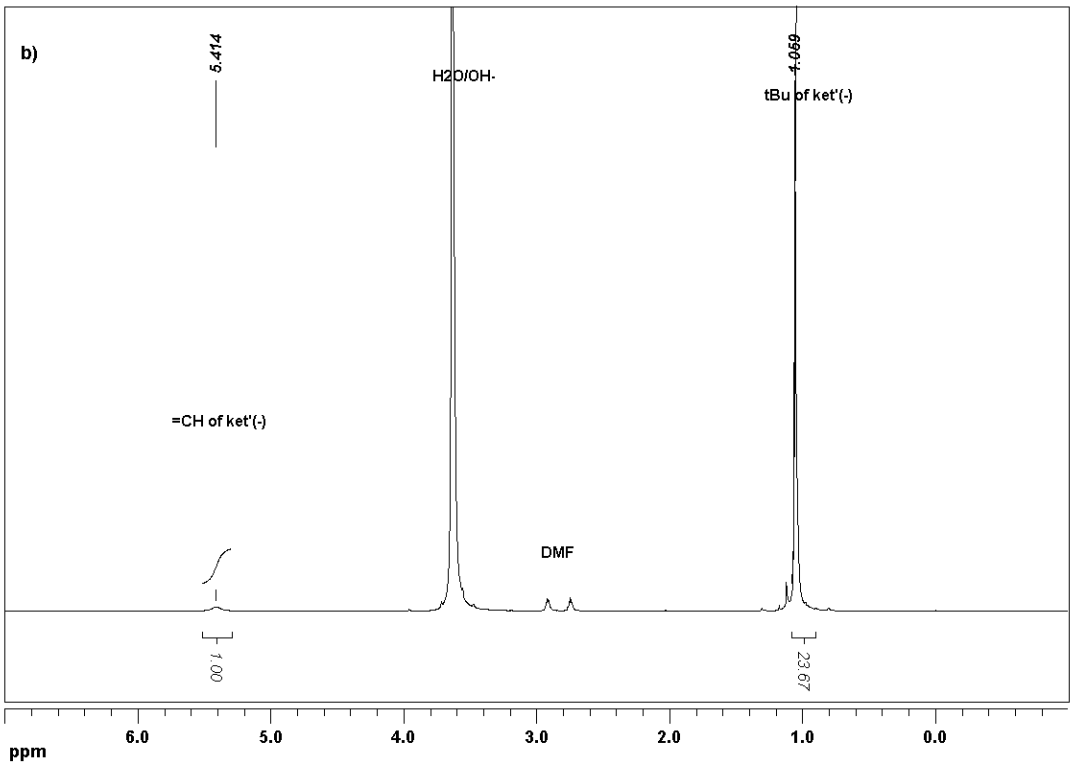
General: ^{1}H-NMR spectra were recorded on a Bruker spectrometer (300 MHz) with TMS as an external reference. ESI/MS spectra were recorded on an API 3000 spectrometer at ENSCP-Paristech. All experiments were performed under argon using Schlenk techniques.

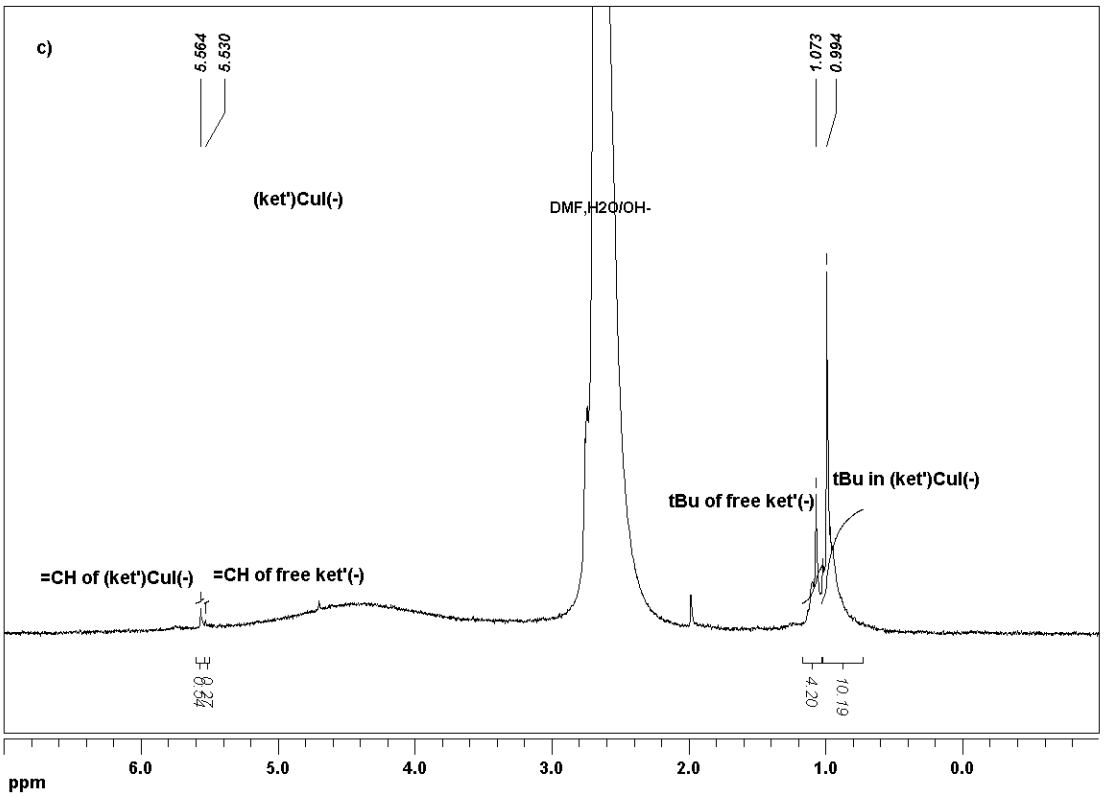
Chemicals. DMF was distilled from calcium hydride under vacuum and kept under argon. Iodobenzene, phenol, 2,2,6,6-tetramethyl-3,5-heptadione (TMHD), PhONa, $CsOH•H_2O$, Cs_2CO_3 and CuI were commercially available and used as received.

I. Characterization of [(ket')Cu-OH]$^-$

a) By ^{1}H NMR.




b)
5.414
H2O/OH-
4.059
tBu of ket'(-)
=CH of ket'(-)
DMF
1.00
23.67
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


c)
5.564
5.530
1.073
0.994
(ket')CuI(-)
DMF,H2O/OH-
tBu of free ket'(-)
tBu in (ket')CuI(-)
=CH of (ket')CuI(-)
=CH of free ket'(-)
0.54
4.20
10.19
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

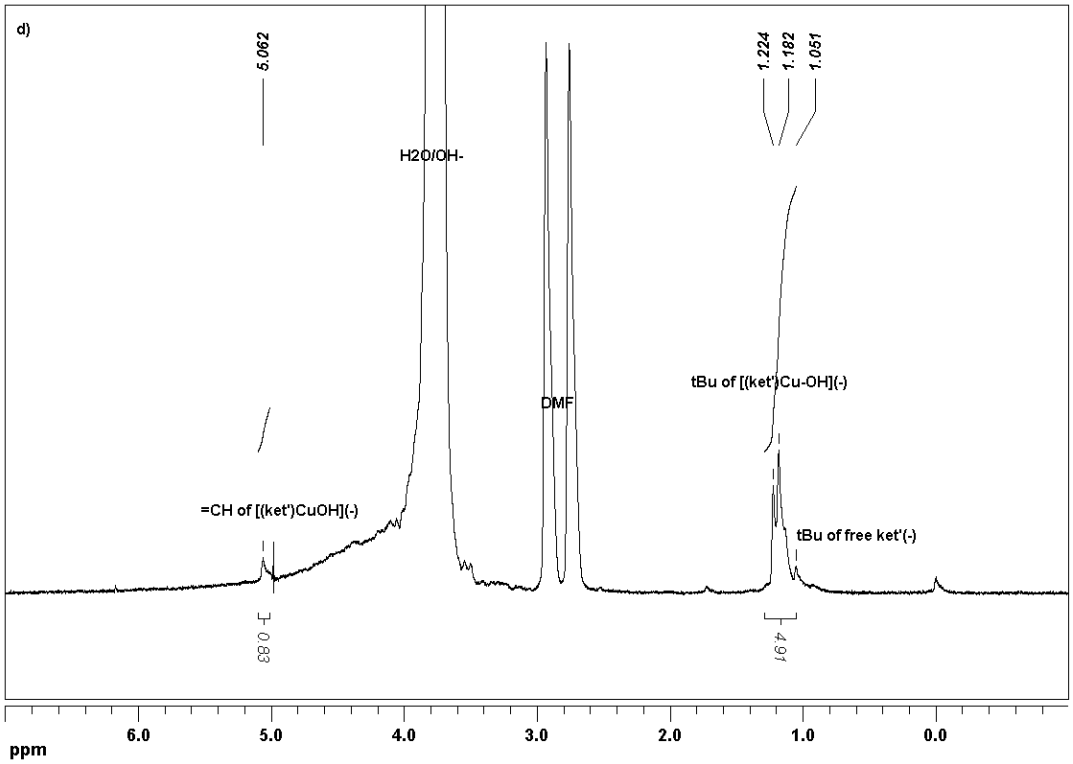
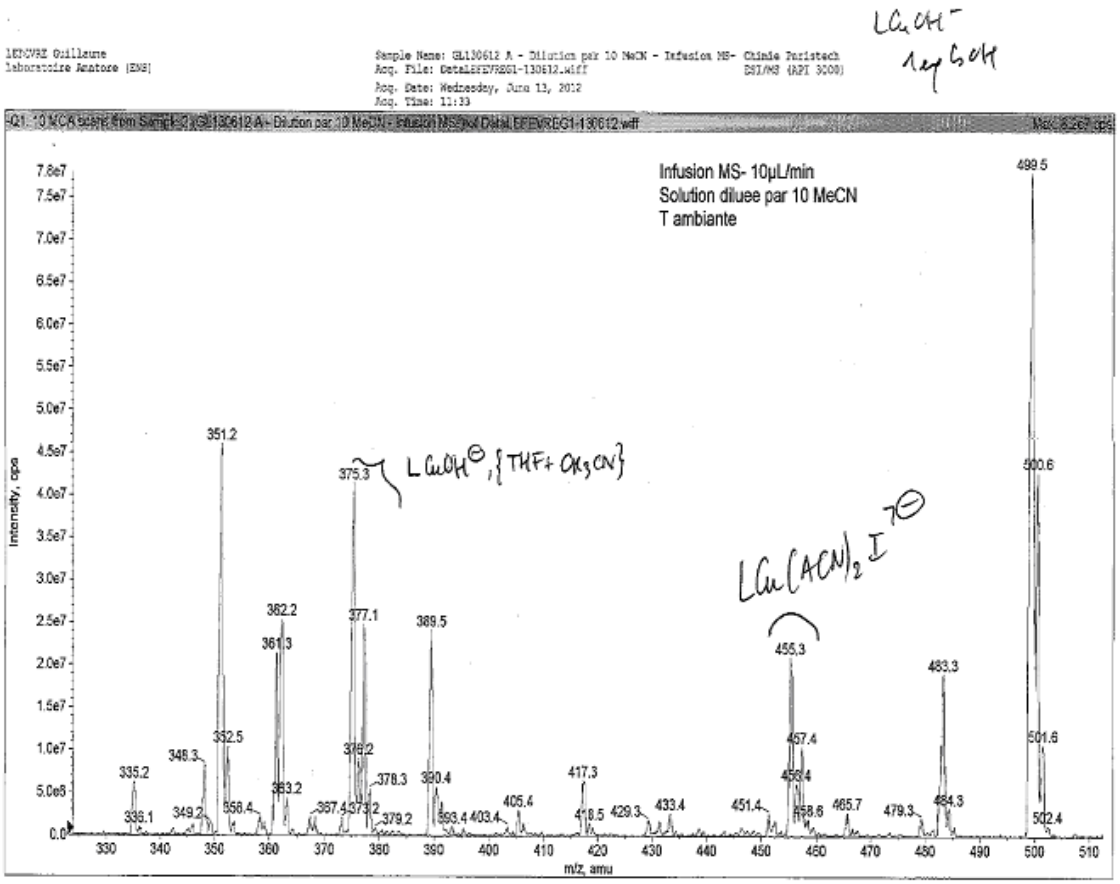


Figure S1. ^{1}H NMR (300 MHz, TMS) in 0.5 mL of DMF-d_7 of a) 2,2,6,6-tetramethyl-3,5-heptanedione (ket'H) (10^{-2} M). b) (ket'H) (10^{-2} M) + CsOH•H_2O (10^{-2} M). c) (ket'H) (10^{-2} M), CsOH•H_2O (10^{-2} M) and CuI (10^{-2} M). d) {(ket'H) (10^{-2} M), CsOH•H_2O (10^{-2} M), CuI (10^{-2} M)} and CsOH•H_2O (10^{-2} M).

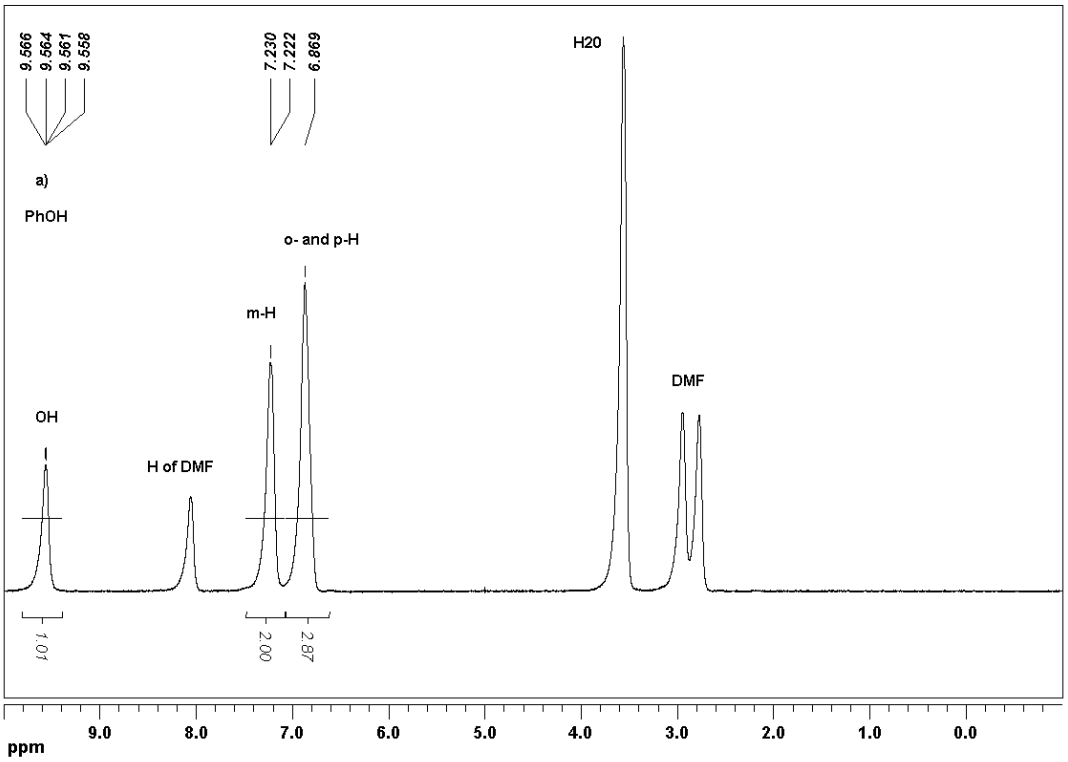
b) By ESI-MS



ESI(-) mass spectrum of complexes formed in the reaction of $CsOH{\bullet}H_2O$ (3.10^{-2} M) with ket'H, $CsOH{\bullet}H_2O$ and CuI (all 3.10^{-2} M) in 2 mL of THF after stirring during 1 h: $[(ket')Cu\text{-}OH]^-$,THF,CH_3CN and $[(ket')CuI]^-$,$2CH_3CN$. The mass peak of ket'^- appeared at 182.6 (L = ket', ACN = acetonitrile)

II. Characterization of [(ket')Cu-OPh]$^-$

a) by ^{1}H NMR



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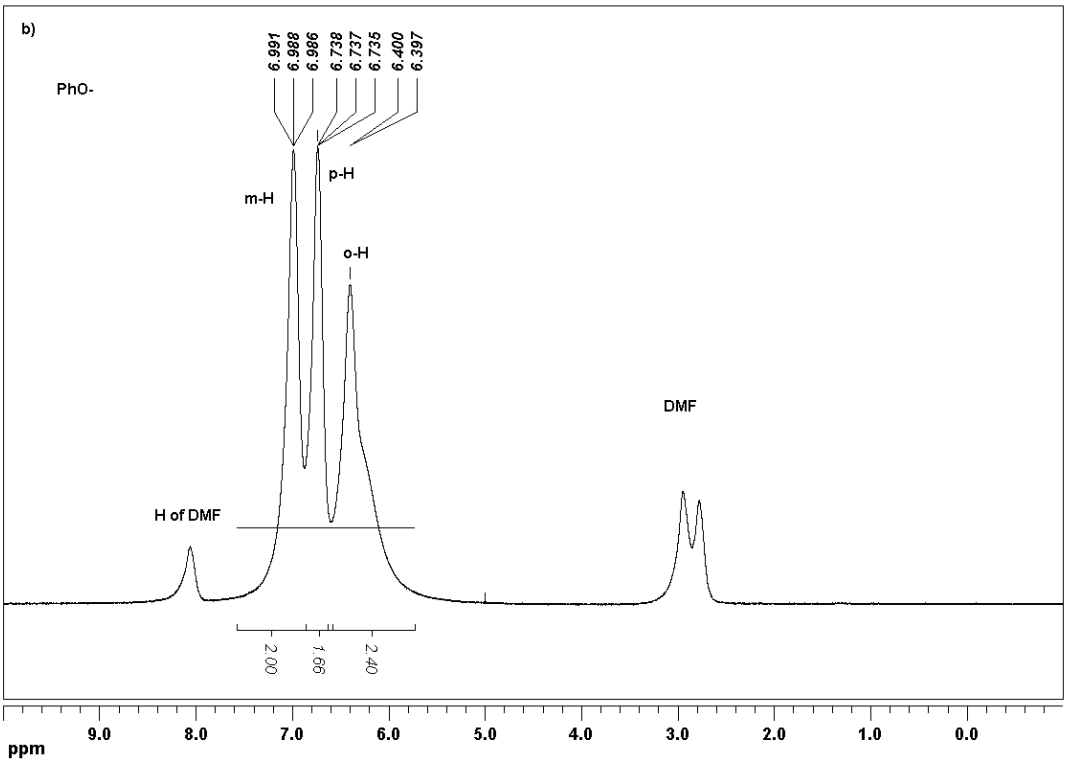

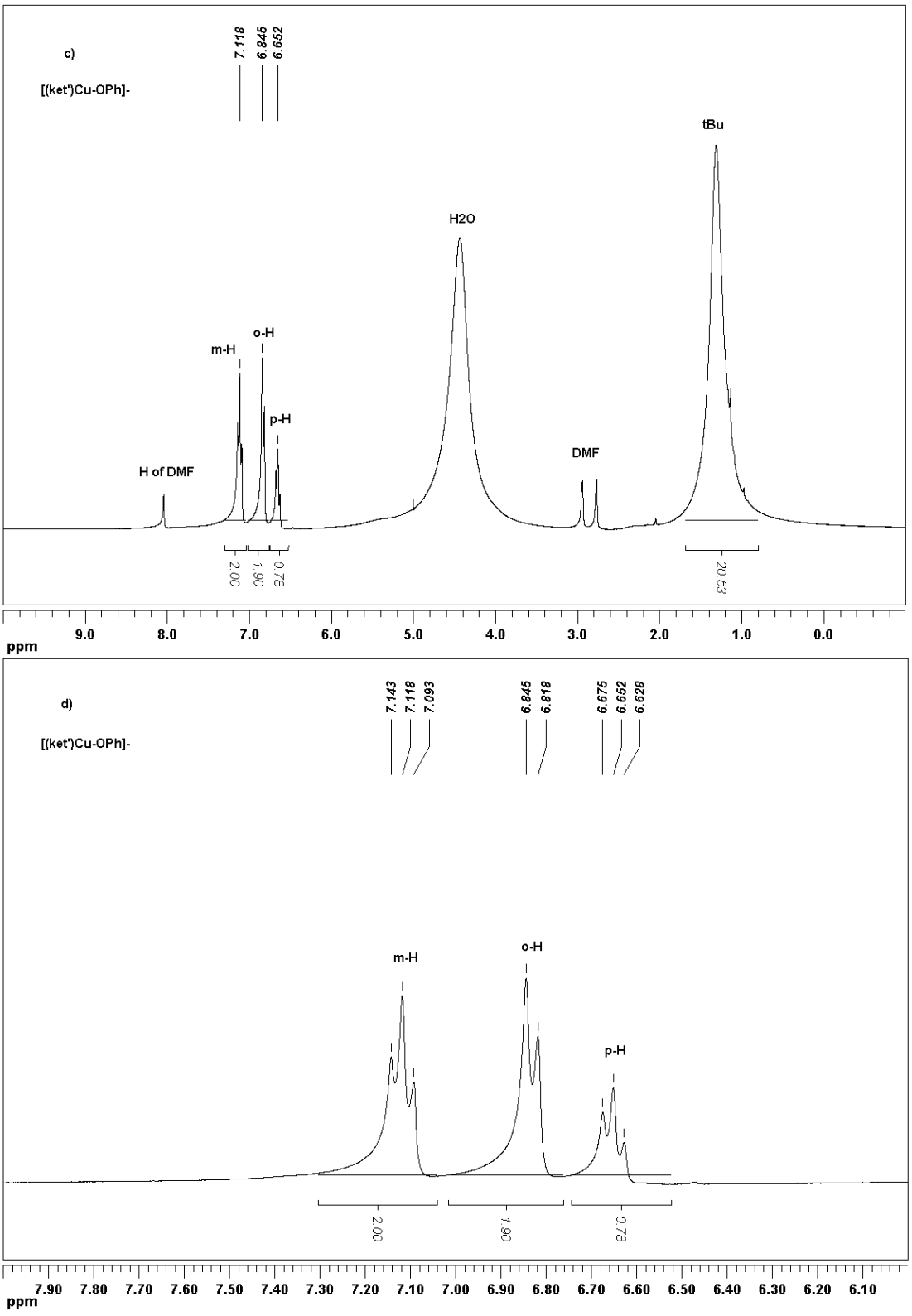

Figure S2. ^{1}H NMR (300 MHz, TMS) in 0.5 mL of DMF-d_7 of a) PhOH (10^{-2} M). b) PhO^- from PhOH (10^{-2} M) and 3 equiv of Cs_2CO_3. c) $[(ket')Cu\text{-}OPh]^-$ from a mother solution of 2 mL of DMF-d_7 containing TMHD (ket'H) (3.10^{-2} M), $CsOH{\bullet}H_2O$ (3.10^{-2} M) and CuI (3.10^{-2} M) to which was added PhOH (3.10^{-2} M) and Cs_2CO_3 (3.10^{-2} M). d) Expanded scale for the aromatic protons of $[(ket')Cu\text{-}OPh]^-$.

b) by ESI-MS

To 2 mL of THF containing ket'H, CsOH and CuI (all 3.10^{-2} M), was added PhOH (3.10^{-2} M) followed by Cs_2CO_3 ($2.2.10^{-2}$ M)). After 1 h, the ESI(-) exhibited the mass peak of $[(ket')Cu\text{-}OPh]^-$: m/z = 339 with the right isotopic pattern for a Cu center (339, 337 as major peaks, 100 % and 45 % respectively). Two other copper complexes were also detected: $[(ket')CuI]^-$,2MeCN (m/z = 455) and $[ICu\text{-}OPh]^-$,THF (m/z = 354).

III. DFT calculations

All calculations were performed using the Gaussian[1a] code (G09 Revision A.02) using density functional theory (DFT) and a hybrid functional, the so-called PBE0[1b] mixing 25% of Hartree-Fock exchange to the gradient corrected PBE exchange and correlation functional[1c] A 6-31+G(d) basis[1d,e] was used for all atoms (C, H, O, N, and I) but the metal (Cu) which was treated using a SDD basis[1f] and associated core pseudopotential.[1g] Solvent effects (here DMF) were introduced using a Continuum Polarizable Model (PCM).[1h] This model which neglects direct solute-solvent interactions, is however fully adequate to model an aprotic polar but weakly coordinating solvent for such as DMF. Computational details are reported in Supporting Information. All structures corresponding to stationary points were fully optimized in absence of geometrical constraints and characterised by subsequent frequencies calculations as minima or first order transition states (i.e. only one imaginary frequency). All molecular orbitals plots were done taking 0.02 as isovalue contour.

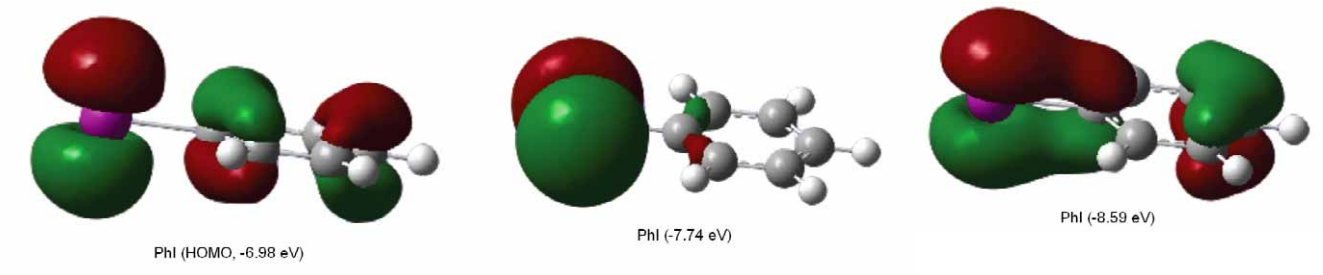

Figure S3: Molecular orbitals of PhI: lone pairs located on the iodine atom

Table S1. Selected computed structural parameters of the optimized structures (distance *d* (in Å) and angle θ (in °)). See Scheme 3 for nomenclature and labelling for the reaction of PhI with [(ket')Cu-OH]$^-$

	(A)	**(B)**	**(E)**	**TS1**	**(F)**	**TSdiss**	**(C)**	**TS2**	**(D)**
d O_1-Cu	1.90								
d O_2-Cu	2.30								
d O-Cu	1.85	1.86	1.96	1.97	1.88	1.88	1.80	1.84	2.00
d Cu-C_1	-	-	2.07	2.18	1.90	1.90	1.90	1.92	3.06
d O-I	-	2.75	3.92	4.24	-	-	-	-	-
d C_1-I*	-	2.13	2.14	2.23	3.14	3.30	-	-	-
d Cu-I	-	3.95	3.37	2.68	2.58	2.73	-	-	-
d C_1-O	-	-	3.21	3.12	2.55	2.55	2.52	1.98	1.38
d Cu-C_{ortho}**	-	-	2.12	2.99	-	-	-	-	-
θ (C_1CuI)	-	8.5	37.7	53.5	87.6	88.8	-	-	-
θ (OCuO_1)	162.6	106.3	110.9	126.2	105.0	129.9	175.1	162.1	144.4
θ (OCuO_2)	109.6	165.2	104.0	98.4	90.0	88.5	89.7	103.6	119.6
θ (CuOI)	-	117.0	59.3	28.3	13.2	27.3	-	-	-
θ (OIC_1)	-	179.4	55.0	45.8	35.0	36.7	-	-	-
θ (IC_1C_{para})	-	179.9	162.2	160.2	130.0	126.4	-	-	-
θ (CuC_1C_{para})	-	-	90.9	125.1	174.9	177.6	177.8	158.0	-
θ (HOCu)	106.4	109.4	105.5	104.1	97.6	97.6	99.3	109.0	119.2
θ (C_1CuO)	-	-	105.7	105.6	84.7	84.9	85.8	-63.5	20.3
θ (C_oCuC_1)**	-	-	39.6	25.9	-	-	-	-	-
θ (O_1O_2OCu)	0.0	-0.15	-50.0	-37.8	-51.8	-34.6	-0.4	-1.8	10.0
θ (O_1O_2CuC_1)	-	.76.6	-114.4	- 105.6	156.3	147.5	- 174.1	179.9	- 179.9
θ (CuOIC_1)	-	144.5	-40.7	98.3	96.8	72.7	-	-	-
θ (HOIC_1)	-	-93.9	-110.2	155.7	164.0	156.1	-	-	-
θ (HOCuO_1)	-180	177.9	64.6	71.8	74.6	81.8	177.8	-97.5	0.1

* *d* C_1-I (in PhI) = 2.12 Å

** C_{ortho} is the carbon atom in the *ortho*-position of PhI when the latter is η^2-ligated onto the copper center in (**E**) and (**TS1)**,

Table S2. Selected computed structural parameters of the optimized structures (distance *d* (Å) and angle θ (°)). See Scheme 6 for nomenclature and labelling for the reaction of PhI with [(ket')Cu-OPh]$^-$ Cu-O_2

	(A')	**(B')**	**(E')**	**TS'1**	**(F')**	**(C')**	**TS'2**	**(D')**
d O_1-Cu	1.92							
d O_2-Cu	2.18							
d O-Cu	1.88	1.90	2.00	2.02	1.93	1.82	1.88	2.02
d Cu-C_1	-	-	2.09	2.08	1.91	1.90	1.95	-
d O-I	-	2.92	3.81	3.30	-	-	-	-
d C_1-I*	-	2.12	3.81	2.30	3.1	-	-	-
d Cu-I	-	3.73	3.35	2.61	2.59	-	-	-
d C_1-O	-	-	3.24	3.02	2.62	2.54	1.91	1.40
d Cu-C_{ortho}***	-	-	2.15	2.93	-	-	-	-
θ (C_1CuI)	-	11.1	38.2	57.4	85.6	-	-	-
θ (OCuO_1)	107.8	150.2	105.2	118.0	109.4	174.0	159.0	129.0
θ (OCuO_2)	162.3	120.2	107.2	99.4	92.3	91.1	106.0	133.8
θ (CuOI)	-	99.4	61.4	24.7	181.1	-	-	-
θ (OIC_1)	-	179.2	12.0	42.1	36.5	-	-	-
θ (IC_1C_{para})	-	179.9	163.2	155.5	129.0	-	-	-
θ (CuC_1C_{para})	-	-	91.4	131.7	174.4	176.6	153.3	-
θ (COCu)**	126.3	126.6	125.1	125.9	118.3	124.3	61.7	116.3
θ (C_1CuO)	-	-	104.6	94.7	85.9	85.9	60.0	25.3
θ (C_oCuC_1)***	-	-	40.0	28.1	-	-	-	-
θ (O_1O_2OCu)	-1.8	1.91	-52.4	-42.5	-48.2	-1.5	-2.6	-0.0
θ (O_1O_2CuC_1)	-	93.3	-119.1	-116.7	-177.6	149.5	-177.0	-
θ (CuOIC_1)	-	-4.7	-38.6	105.1	87.4	-	-	-
θ (COIC_1)**	-	-144.1	74.6	126.1	80.9	-	-	-
θ (COCuO_1)**	-172.1	161.9	155.5	40.8	2.99	-93.0	-12.7	179.8

* *d* C_1-I (in PhI) = 2.12

** "C" is the carbon atom linked to the O of phenoxy group in (**A'**), (**B'**), (**E'**), (**TS1'**), (**F'**), (**C'**), (**TS2'**), (**D'**).

*** C_{ortho} is the carbon atom in the *ortho*-position of PhI when the latter is η^2-ligated onto the copper center in (**E**') and **TS1'**.

Table S3. Spin Multiplicity and Negative Frequencies /cm^{-1}

	(A)	**(B)**	**(B'')**	**(E)**	**TS1**	**(F)**	**(TSdiss)**	**(C)**	**(TS2)**	**(D)**
Spin multiplicity	1	1	1	1	1	1	1	1	1	1
Negative frequencies /cm^{-1}	-	-	-	-	-93.4	-	-68.2	-	-301.0	-

	(A')	**(B')**	**(E')**	**TS'1**	**(F')**	**(C')**	**(TS'2)**	**(D')**
Spin multiplicity	1	1	1	1	1	1	1	1
Negative frequencies /cm^{-1}	-	-	-	-62.5	-	-	-305.3	-

Table S4. Selected computed structural parameters of the optimized structures (distance *d* (Å) and angle θ(°)) for complex **B''** (See Fig 2 for labelling).

	(B'')
d O_1-Cu	1.86
d O_2-Cu	2.26
d O-Cu	1.85
d C_1-I *	2.14
d Cu-C_1	5.31
d Cu-I	3.18
θ (C_1CuI)	1.96
θ (OCuO_1)	168.0
θ (OCuO_2)	102.6
θ (CuOI)	65.5
θ (OIC$_1$)	152.8
θ (IC$_1$C$_{para}$)	179.9
θ (HOCu	103.8
θ (O_1O_2OCu)	0.2
θ (O_1O_2CuC$_1$)	22
θ (CuO_1C$_1$)	-179.3
θ (HOIC_1)	165.5
θ (HOCuO_1)	-178.8

* *d* C_1-I (in PhI) = 2.12 Å

Cartesian coordinates of computed structures (in Ångströms). The most stable spin multiplicities are given between parenthesis.

Complex [(ket')CuI]$^{-}$ (1)

Cu	-1.0829330	-0.0005390 -0.0001940
O	0.3031590	-1.4603990 -0.0001310
C	1.5563010	-1.2633170 -0.0001570
C	2.1827570	0.0002360 -0.0002870
C	1.5558220	1.2635250 -0.0002890
O	0.3025910	1.4601060 -0.0004850
C	2.4568460	2.5191140 0.0000550
H	3.2670350	0.0004440 -0.0001830
C	2.4578000	-2.51851900.0000350
C	1.6039730	-3.78760100.0002000
H	0.9604070	-3.8399360-0.8842210
H	2.2588350	-4.66763600.0003330
H	0.9603870	-3.83968700.8846210
C	3.3449590	-2.51978001.2554580
H	3.9573550	-3.43038801.2770110
H	4.0228340	-1.66014901.2820130
H	2.7369760	-2.50061202.1681460
C	3.3450650	-2.5201790-1.2553060
H	3.9574930	-3.4307740-1.2764930
H	2.7371570	-2.5013510-2.1680520
H	4.0229170	-1.6605410-1.2821120
C	1.6024890	3.7878410 -0.0006730
H	0.9582820	3.8398790 0.8832950
H	2.2569910	4.6681450 -0.0003300
H	0.9595030	3.8396730 -0.8855480
C	3.3449160	2.5208250 -1.2546920
H	4.0232590	1.6615490 -1.2808090
H	2.7376240	2.5013870 -2.1678370
H	3.9568990	3.4317240 -1.2757890
C	3.3431440	2.5210220 1.2560730
H	3.9552850	3.4318010 1.2777910
H	2.7345540	2.5019510 2.1683590
H	4.0212320	1.6615770 1.2833380
I	-3.5601960	-0.00015200.0000850

Complex A (1)

Cu	-0.37998902.3234960	0.0000550
O	1.4436860	0.9136720 -0.0003070
C	1.3235430	-0.3357560-0.0001820
C	0.0812200	-1.0277520-0.0000500
C	-1.2017620	-0.46635900.0001110
O	-1.48162600.7790300	0.0003220
C	-2.4148890	-1.4255200-0.0000380
O	0.1951250	4.0822900 -0.0000960
H	1.1626820	4.0534770 -0.0006200
H	0.1294860	-2.1111440-0.0001400
C	2.6140080	-1.1928720-0.0000050
C	3.8467760	-0.2887710-0.0006970
H	3.8706620	0.3576650 0.8830010
H	4.7546800	-0.9047180-0.0004840
H	3.8704090	0.3566630 -0.8851460
C	2.6495460	-2.0795540-1.2547280
H	3.5833120	-2.6563470-1.2781320
H	1.8168850	-2.7903520-1.2807260
H	2.6056020	-1.4731000-2.1678130
C	2.6497630	-2.07798801.2558670
H	3.5834160	-2.65494601.2797370
H	2.6061930	-1.47035702.1681810
H	1.8169180	-2.78852901.2829430
C	-3.7252790	-0.63560400.0005930
H	-3.81074000.0044550	-0.8836850
H	-4.5710050	-1.33449400.0004140
H	-3.81038100.0035760	0.8855420
C	-2.3765860	-2.31320701.2544460
H	-1.4854040	-2.94886501.2820670
H	-2.3877240	-1.70558502.1675150
H	-3.2571160	-2.96831001.2740900
C	-2.3769980	-2.3119900-1.2554010
H	-3.2575240	-2.9670880-1.2754180
H	-2.3884010	-1.7034870-2.1678800
H	-1.4857990	-2.9475940-1.2838840

Complex B (1)

Cu	1.1376440	-1.3879030	-0.8677500
O	1.3832470	0.8624400	-0.8408750
C	2.3941810	1.4293610	-0.3575890
C	3.4858350	0.7510450	0.2492780
C	3.6331900	-0.63220100	.4132540
O	2.8061520	-1.52825600	.0357950
C	4.9107170	-1.15030801	.1132630
O	-0.4770290	-1.7272400	-1.7219650
H	-0.6093630	-2.6828940	-1.7895980
H	4.2929080	1.3682250	0.6284880
C	2.4632080	2.9750450	-0.4241130
C	1.2110630	3.5294080	-1.1040270
H	0.3027900	3.2532250	-0.5581660
H	1.2687950	4.6244040	-1.1436800
H	1.1109660	3.1540880	-2.1278290
C	3.6972550	3.4045290	-1.2330910
H	3.7260380	4.4986500	-1.3174790
H	4.6320950	3.0804810	-0.7635610
H	3.6666500	2.9896610	-2.2482100
C	2.5522990	3.5540700	0.9965810
H	2.5627090	4.6508380	0.9518550
H	1.6889330	3.2500430	1.6012280
H	3.4600770	3.2316700	1.5173150
C	4.8891570	-2.67701501	.2105150
H	4.8434930	-3.14376800	.2211560
H	5.8025080	-3.02250501	.7106490
H	4.0285640	-3.03173901	.7871690
C	4.9985980	-0.56953102	.5336120
H	5.0747260	0.5227610	2.5273890
H	4.1179150	-0.84445503	.1267970
H	5.8863170	-0.96548603	.0435030
C	6.1504070	-0.72657800	.3090200
H	7.0568260	-1.12361800	.7839990
H	6.1078440	-1.1168200	-0.7151960
H	6.2508830	0.3623720	0.2522180
I	-2.7462640	-0.7581280	-0.5104200
C	-4.5171920	-0.00120400	.4103160
C	-5.63292600	.3141790	-0.3692060
C	-4.55964900	.1797980	1.7950850
C	-6.78755100	.8100860	0.2389250
H	-5.60687400	.1759670	-1.4468250
C	-5.71774800	.6763500	2.3958590
H	-3.6953150	-0.06366102	.4072460
C	-6.83385100	.9927710	1.6211250
H	-7.65230501	.0537640	-0.3736890
H	-5.74365800	.8151220	3.4740650
H	-7.73414101	.3792660	2.0916600

Complex E (1)

Cu	0.4274110	-0.66033100	.7227150
O	-1.5476710	-1.28458700	.6767640
C	-2.5782420	-0.68068900	.2502910
C	-2.64613900	.6838000	-0.0828980
C	-3.8339510	-1.57375000	.1086170
C	-1.59497301	.6328050	0.0295390
O	-0.42943701	.3795240	0.4259960
C	-1.91617103	.0966120	-0.3651140
C	2.1597400	-0.8648680	-0.3929380
C	2.7408130	-2.1378650	-0.1507230
C	1.0710430	-0.7446680	-1.2981290
C	2.2163890	-3.2596660	-0.7636730
H	3.5925200	-2.22386100	.5167970
C	0.5742510	-1.9156110	-1.9204250
H	0.7399770	0.2313850	-1.6398790
C	1.1297250	-3.1527060	-1.6551870
H	2.6578630	-4.2318890	-0.5594620
H	-0.2476000	-1.8203850	-2.6256930
H	0.7406330	-4.0419870	-2.1437620
I	3.3600930	0.8569400	0.0511100
H	-3.59695401	.0579190	-0.4386250
C	-0.67683903	.9752560	-0.1932070
H	0.1503870	3.6284570	-0.8216140
H	-0.91588005	.0075290	-0.4786080
H	-0.32703003	.9783640	0.8444570
C	-2.35970103	.1531470	-1.8355110
H	-3.27945902	.5854880	-2.0111770
H	-2.54635604	.1943970	-2.1291810
H	-1.58235202	.7512760	-2.4972850
C	-3.03795703	.6439640	0.5312760
H	-2.75614303	.5928940	1.5902270
H	-3.23310204	.6959110	0.2850670
H	-3.97426303	.0905990	0.4038600
C	-5.0892710	-0.8388110	-0.3657890
H	-5.3855080	-0.04187100	.3267170
H	-4.9580010	-0.3990180	-1.3616330
H	-5.9238540	-1.5486220	-0.4278650
C	-3.5060240	-2.6863270	-0.8988080
H	-2.6237950	-3.2515410	-0.5827570
H	-4.3521170	-3.3801990	-0.9833930
H	-3.3089360	-2.2713530	-1.8956450
C	-4.1215290	-2.20321201	.4796840
H	-4.9697530	-2.89586301	.4071230
H	-3.2508190	-2.75657801	.8440990
H	-4.3755300	-1.43501202	.2212980
O	0.9660550	-0.92749002	.5878750
H	0.1476600	-0.88827403	.1022540

TS1 (1)

Negative frequency: -93,4 cm^{-1}

Cu	-0.6144280	-0.4722890	-0.8459860
O	0.3409800	1.3773010	-0.4267290
C	1.5500570	1.5712920	-0.1012480
C	2.5586180	0.5886990	-0.0818450
C	1.8849780	3.0269730	0.3044090
C	2.4160540	-0.7687690	-0.4620660
O	1.3522200	-1.2981830	-0.8816990
C	3.6691870	-1.6735080	-0.3664960
C	-2.5846260	-0.10691500	0.0203290
C	-2.68834201.2904290		0.0753100
C	-3.5685110	-0.8729520	-0.6217220
C	-3.73455501.9190980		-0.5984830
H	-1.94005701.8726420		0.6013510
C	-4.6077590	-0.2252270	-1.2824450
H	-3.5070970	-1.9561640	-0.6245460
C	-4.69625001.1693360		-1.2769490
H	-3.79917103.0045290		-0.5801760
H	-5.3579980	-0.8185110	-1.7998890
H	-5.51656801.6664560		-1.7877610
I	-1.4125420	-1.12151101.6251420	
H	3.5442080	0.8977940	0.2403550
C	3.3298200	-3.0985670	-0.8052990
H	2.9829680	-3.1275340	-1.8435470
H	4.2233210	-3.7301830	-0.7240120
H	2.5435460	-3.5340340	-0.1796330
C	4.7766280	-1.1257840	-1.2808580
H	5.1078660	-0.1280040	-0.9746000
H	5.6481110	-1.7926910	-1.2512610
H	4.4348040	-1.0647600	-2.3214530
C	4.1741600	-1.71173801.0843140	
H	4.4804660	-0.72263801.4403670	
H	3.3991590	-2.09057001.7619620	
H	5.0422330	-2.37963701.1593220	
C	1.5178040	3.9386390	-0.8759160
H	0.4668840	3.8122200	-1.1532350
H	1.6834050	4.9896920	-0.6072040
H	2.1349810	3.7140970	-1.7552980
C	1.0104000	3.3891000	1.5139500
H	-0.05021103.2514330		1.2818060
H	1.2566450	2.7640690	2.3818770
H	1.1699400	4.4374680	1.7965660
C	3.3511110	3.2657930	0.6703660
H	3.6621010	2.6694730	1.5363770
H	4.0244640	3.0390100	-0.1647440
H	3.4935830	4.3221490	0.9311620
O	-1.2181920	-1.0937170	-2.6130160
H	-0.3971560	-1.2984440	-3.0832780

Complex F (1)

Cu	-0.7208570	-0.4869660	-0.6856780
O	0.2608940	1.4853390	-0.3640640
C	1.4794860	1.6220160	-0.0820450
C	2.4376320	0.5789930	-0.1316330
C	1.9150110	3.0491960	0.3216020
C	2.2026940	-0.7400970	-0.5415560
O	1.0734570	-1.2393670	-0.8591260
C	3.4025830	-1.7084600	-0.6224110
I	-0.9882310	-1.1362950	1.7966650
C	-2.5499490	0.0283720	-0.6646730
C	-3.5452840	-0.9007120	-0.9416770
C	-2.8369070	1.3752630	-0.4850310
C	-4.8700390	-0.4647260	-1.0357760
H	-3.3080190	-1.9513900	-1.0828720
C	-4.1677110	1.7993350	-0.5846550
H	-2.0425890	2.0860470	-0.2750940
C	-5.1836150	0.8839900	-0.8576200
H	-5.6557050	-1.1863410	-1.2494980
H	-4.4022660	2.8529770	-0.4476260
H	-6.2153050	1.2188540	-0.9321970
H	3.4588080	0.8267540	0.1240040
C	2.9691250	-3.0598690	-1.1936660
H	2.5650370	-2.9578510	-2.2066010
H	3.8371170	-3.7289290	-1.2378920
H	2.2023960	-3.5339080	-0.5730970
C	4.5021390	-1.1245720	-1.5224360
H	4.1229070	-0.9292680	-2.5327630
H	4.9104410	-0.1890180	-1.1269930
H	5.3290650	-1.8411110	-1.6051400
C	3.9557810	-1.9236410	0.7964170
H	4.3346590	-0.9930490	1.2320030
H	3.1820700	-2.3214660	1.4642200
H	4.7817960	-2.6455990	0.7670820
C	3.3957690	3.1846320	0.6816000
H	3.6720100	2.5500480	1.5320820
H	4.0498690	2.9361830	-0.1625360
H	3.6057470	4.2235730	0.9646200
C	1.0707160	3.4692230	1.5341410
H	1.3023050	4.5050790	1.8120380
H	0.0022090	3.4007160	1.3084450
H	1.2800620	2.8318570	2.4025320
C	1.6035850	3.9793980	-0.8605280
H	1.8415960	5.0172380	-0.5955520
H	2.1983500	3.7107730	-1.7427730
H	0.5444860	3.9243430	-1.1304300
O	-0.9558440	-0.6153200	-2.5427580
H	-0.0301250	-0.7961470	-2.7772880

TSdiss (1)

Negative frequency: -62,8 cm^{-1}

Cu	-0.6323220	-0.4962960	-0.7433940
O	0.1315950	1.3940850	-0.3407710
C	1.3405830	1.6444620	-0.0583390
C	2.3895610	0.7067250	-0.1087650
C	1.6159850	3.1063290	0.3477780
C	2.2685610	-0.6224690	-0.5442820
O	1.1809610	-1.1956620	-0.8697090
C	3.5403210	-1.4855560	-0.6493680
I	-0.9551370	-1.22566901	.8733130
C	-2.46264900	.0321720	-0.7789960
C	-3.4527230	-0.9140870	-1.0120940
C	-2.75796701	.3799940	-0.6311650
C	-4.7837250	-0.4957840	-1.0816060
H	-3.1981840	-1.9602750	-1.1464560
C	-4.09678501	.7868200	-0.7129490
H	-1.96916602	.1043570	-0.4532330
C	-5.10833900	.8545510	-0.9336770
H	-5.5658520	-1.2314840	-1.2569290
H	-4.33790202	.8419890	-0.6013210
H	-6.14509901	.1766660	-0.9932990
H	3.3818870	1.0469700	0.1516520
C	3.2107960	-2.8654560	-1.2215780
H	2.7823300	-2.7925860	-2.2269050
H	4.1303560	-3.4595410	-1.2850590
H	2.4977270	-3.4047310	-0.5901960
C	4.5679780	-0.8021480	-1.5649930
H	4.1569850	-0.6418410	-2.5689240
H	4.8944080	0.1664520	-1.1731910
H	5.4548020	-1.4407400	-1.6611450
C	4.1336250	-1.65849800	.7591100
H	4.4375200	-0.70174901	.1965590
H	3.4100670	-2.12829201	.4360810
H	5.0193960	-2.30388500	.7084060
C	3.0797120	3.3982040	0.6825940
H	3.4359840	2.7977390	1.5278450
H	3.7413340	3.2203100	-0.1732510
H	3.1815300	4.4535610	0.9633070
C	0.7514270	3.4198960	1.5787530
H	0.8818760	4.4701680	1.8671030
H	-0.30813403	.2474210	1.3671070
H	1.0378700	2.7960580	2.4344270
C	1.1820640	4.0051870	-0.8203170
H	1.3183860	5.0594410	-0.5498580
H	1.7814450	3.8059060	-1.7174230
H	0.1283500	3.8438560	-1.0674620
O	-1.0113730	-1.3163670	-2.3916550
H	-0.1083220	-1.6112440	-2.5985530

Complex C (1)

Cu	0.6679820	-1.0079820 -0.0505900
O	0.3954920	0.8281240 -0.0025330
C	-0.75279401.4078110	0.0719260
C	-1.98800000.7661310	0.0776450
C	-0.63958102.9357270	0.1445540
C	-2.1644100	-0.6284090 -0.0150870
O	-1.2049100	-1.4583710 -0.0738360
C	-3.5814750	-1.2102930 -0.0478080
C	2.5447830	-0.7080700 -0.0466820
C	3.3460330	-1.34593400.8886640
C	3.0544340	0.1820540 -0.9822600
C	4.7146000	-1.05528200.9016220
H	2.9268060	-2.06382601.5867060
C	4.4295020	0.4427210 -0.9724300
H	2.4104540	0.6793200 -1.7017110
C	5.2554760	-0.1682700 -0.0294230
H	5.3551300	-1.53583401.6375530
H	4.8461580	1.1318720 -1.7033930
H	6.3214270	0.0445570 -0.0220040
H	-2.87592201.3785710	0.1372680
C	-3.5359320	-2.7351500 -0.1589490
H	-3.0144290	-3.18652900.6912910
H	-4.5601450	-3.1247160 -0.1779630
H	-3.0313640	-3.0580230 -1.0754200
C	-4.3119190	-0.81977301.2484680
H	-3.7834640	-1.19863502.1309030
H	-4.41876100.2647300	1.3525320
H	-5.3172950	-1.25726001.2419200
C	-4.3349020	-0.6379700 -1.2604360
H	-4.44551600.4496550	-1.2034670
H	-3.8206740	-0.8817270 -2.1972860
H	-5.3393160	-1.0759740 -1.3015820
C	0.2155990	3.2887320	1.3727130
H	1.2066960	2.8306890	1.3080190
H	0.3383730	4.3764490	1.4322510
H	-0.26363702.9509170	2.2995500
C	0.0711440	3.4172650	-1.1311070
H	1.0611350	2.9620170	-1.2274470
H	-0.51340603.1728590	-2.0262630
H	0.1930850	4.5061330	-1.0934120
C	-1.99225903.6402710	0.2579960
H	-2.63088003.4491420	-0.6119550
H	-2.53567903.3455260	1.1631020
H	-1.82523704.7221690	0.3112950
O	1.0815180	-2.7629500 -0.0777460
H	0.1863910	-3.1343800 -0.1668980

TS2 (1)

Negative frequency: -300,1 cm^{-1}

Cu	0.6985560	-1.0123010	-0.0045640
O	0.3611000	0.8452280	-0.0137600
C	-0.79721801.4013910		-0.0042460
C	-2.01892200.7276530		0.0018960
C	-0.73240002.9361010		-0.0010660
C	-2.1832200	-0.67771300.0000700	
O	-1.2252290	-1.5050420	-0.0030640
C	-3.6081070	-1.25351000.0036760	
C	2.6135190	-0.9643160	-0.0028590
C	3.2299280	-0.72714001.2221940	
C	3.2374150	-0.7075670	-1.2197600
C	4.5021630	-0.15456201.2183190	
H	2.7370430	-0.97739002.1572760	
C	4.5159770	-0.1420800	-1.1965070
H	2.7477670	-0.9174880	-2.1669900
C	5.1488380	0.1361110	0.0145650
H	4.9914800	0.0537170	2.1667480
H	5.0116430	0.0799490	-2.1385130
H	6.1446070	0.5705600	0.0220450
H	-2.91843901.3272480		0.0082250
C	-3.5671940	-2.7824190	-0.0037670
H	-3.0481610	-3.17555200.8764280	
H	-4.5920930	-3.17194600.0001390	
H	-3.0583440	-3.1670960	-0.8936710
C	-4.3459640	-0.77876301.2666840	
H	-3.8203460	-1.09677702.1749250	
H	-4.45291200.3103620		1.2985340
H	-5.3518890	-1.21561001.2881940	
C	-4.3589470	-0.7669750	-1.2470550
H	-4.46796300.3222170		-1.2669610
H	-3.8418970	-1.0749340	-2.1636550
H	-5.3644340	-1.2050830	-1.2631610
C	0.0521010	3.3713540	1.2473490
H	1.0524980	2.9286240	1.2566900
H	0.1549870	4.4630320	1.2580510
H	-0.46792903.0716420		2.1655630
C	0.0286110	3.3780210	-1.2615770
H	1.0287050	2.9355510	-1.2920760
H	-0.50871203.0833320		-2.1714290
H	0.1314220	4.4697540	-1.2683410
C	-2.10406303.6126180		0.0134640
H	-2.69831403.3587640		-0.8720820
H	-2.68254603.3523530		0.9075610
H	-1.96635204.7003440		0.0160440
O	1.5608460	-2.63590400.0845380	
H	1.7332200	-2.9523330	-0.8171830

Complex D (1)

Cu	-0.4653900	-1.0726670	0.0052450
O	1.3839690	-1.6389980	0.0037680
C	2.3698660	-0.8259500	-0.0011320
C	2.2793910	0.5745040	-0.0030470
C	3.7468890	-1.5186650	-0.0035620
C	1.1062980	1.3698090	0.0005880
O	-0.0787880	0.9258050	0.0042220
C	1.2787750	2.9038020	0.0002580
H	3.2146770	1.1172630	-0.0068430
C	-0.0869280	3.5925810	0.0043050
H	-0.6711140	3.3238130	0.8907000
H	0.0540040	4.6803150	0.0040990
H	-0.6761570	3.3241450	-0.8788480
C	2.0560930	3.3367570	1.2540650
H	3.0676460	2.9181380	1.2777900
H	2.1450370	4.4302440	1.2747340
H	1.5373620	3.0233080	2.1681220
C	2.0488630	3.3373830	-1.2577560
H	3.0602490	2.9187550	-1.2876260
H	1.5247940	3.0245330	-2.1689670
H	2.1377850	4.4308760	-1.2782930
C	3.8332590	-2.3945950	1.2564870
H	3.0112450	-3.1159950	1.2875850
H	4.7809980	-2.9470140	1.2642120
H	3.7910300	-1.7833150	2.1667050
C	3.8193080	-2.4153070	-1.2497750
H	2.9972420	-3.1372060	-1.2596480
H	3.7665040	-1.8190490	-2.1693790
H	4.7671390	-2.9675350	-1.2591730
C	4.9380020	-0.5585870	-0.0181330
H	4.9443650	0.0765380	-0.9117980
H	4.9572450	0.0878150	0.8671940
H	5.8683800	-1.1394790	-0.0210160
O	-2.3597990	-1.7105070	0.0051370
C	-3.5334830	-0.9798810	0.0012040
C	-4.7697210	-1.6190760	-0.0029320
C	-3.4306350	0.4075120	0.0014850
C	-5.9293170	-0.8442180	-0.0067680
H	-4.8313770	-2.7052030	-0.0034610
C	-4.5998060	1.1663140	-0.0023680
H	-2.4492190	0.8769620	0.0045350
C	-5.8511010	0.5481330	-0.0064740
H	-6.8969400	-1.3388230	-0.0100770
H	-4.5272170	2.2507890	-0.0021800
H	-6.7575460	1.1468140	-0.0094960
H	-2.5374170	-2.6628560	0.0053410

Cs2CO3 (1)

C	-0.2817650	0.1259760	0.2497790
O	-0.9778260	1.2168900	0.1778320
O	1.0135240	0.1757410	0.2555870
O	-0.8890880	-1.0179340	0.3114120
Cs	3.8707070	-0.0308680	-0.0617220
Cs	-3.7158390	-0.0373760	-0.0738650

CsHCO3 (1)

C	2.1719810	0.0459010	-0.0000190
O	1.6010480	1.1591390	-0.0000460
O	3.5402900	0.0581170	0.0000600
O	1.6347010	-1.0969990	-0.0000530
H	3.8550730	-0.8439330	0.0000750
Cs	-1.2926410	-0.0071550	0.0000060

Complex A' (1)

Cu	0.8127510	-0.0872930	-0.0881080
O	-0.8285820	-1.5272320	-0.0380540
C	-2.0438970	-1.1905330	0.0068430
C	-2.5102510	0.1456570	0.0093580
C	-3.0555580	-2.3591080	0.0655140
C	-1.7228190	1.3105060	-0.0229190
O	-0.4511870	1.3530970	-0.0593640
C	-2.4451210	2.6761800	-0.0134280
H	-3.5812720	0.2948210	0.0423520
C	-1.4294890	3.8203310	-0.0376950
H	-0.8008730	3.7820610	-0.9333370
H	-1.9619490	4.7795180	-0.0331640
H	-0.7695380	3.7915620	0.8356080
C	-3.3471260	2.7915730	-1.2528970
H	-4.1292750	2.0254720	-1.2641660
H	-3.8367150	3.7737920	-1.2662060
H	-2.7628330	2.6934740	-2.1759640
C	-3.3003800	2.8048950	1.2573400
H	-4.0873980	2.0450500	1.3033250
H	-2.6835200	2.7089930	2.1591780
H	-3.7826140	3.7905280	1.2816970
C	-2.8411830	-3.2247830	-1.1850750
H	-1.8035290	-3.5664680	-1.2483880
H	-3.4957460	-4.1050020	-1.1526080
H	-3.0749660	-2.6640190	-2.0990660
C	-2.7323950	-3.1881970	1.3176430
H	-1.6927140	-3.5293610	1.3006260
H	-2.8863000	-2.6000150	2.2313640
H	-3.3871160	-4.0674040	1.3679970
C	-4.5234060	-1.9313330	0.1235550
H	-4.7416690	-1.3302790	1.0143080
H	-4.8207830	-1.3571620	-0.7620730
H	-5.1603270	-2.8238390	0.1655100
O	2.4255890	-1.0557490	-0.1489990
C	3.6371530	-0.5547780	-0.0538530
C	4.7642970	-1.4117680	-0.1397760
C	3.9010990	0.8240780	0.1376050
C	6.0615780	-0.9176440	-0.0404460
H	4.5894300	-2.4760810	-0.2864820
C	5.2035740	1.3084680	0.2359910
H	3.0509980	1.5026180	0.2073600
C	6.3012790	0.4475860	0.1489490
H	6.8995730	-1.6095760	-0.1116210
H	5.3625240	2.3757150	0.3834970
H	7.3161280	0.8293900	0.2264530

Complex B'(1)

Cu	0.9319280	0.2905440	-0.4858600
O	1.3894740	-1.5809620	-0.3918790
C	2.5156480	-2.1338310	-0.1512370
C	3.7141430	-1.4626350	0.1185800
C	2.4681230	-3.6755740	-0.1718620
C	3.8985880	-0.0541680	0.1807410
O	2.9920320	0.7973150	-0.0054480
C	5.3192690	0.4669400	0.5022720
H	4.5885660	-2.0720940	0.3033940
C	5.3272020	1.9955170	0.5355210
H	4.6448340	2.3843100	1.2988610
H	6.3388250	2.3520220	0.7660220
H	5.0259040	2.4201750	-0.4278320
C	5.7678280	-0.0606720	1.8744970
H	5.8352820	-1.1534130	1.8945830
H	6.7589580	0.3413860	2.1207950
H	5.0722990	0.2507090	2.6634500
C	6.3019980	-0.0114080	-0.5784070
H	6.3774170	-1.1033900	-0.6128730
H	5.9967150	0.3388620	-1.5720370
H	7.3036710	0.3878250	-0.3732470
C	1.4721520	-4.1282870	0.9077600
H	0.4862720	-3.6832270	0.7417240
H	1.3679820	-5.2205390	0.8887460
H	1.8168020	-3.8392050	1.9086150
C	1.9522130	-4.1150560	-1.5509600
H	0.9746180	-3.6712460	-1.7613630
H	2.6457370	-3.8143690	-2.3464750
H	1.8529100	-5.2073210	-1.5843960
C	3.8152140	-4.3525150	0.0875370
H	4.5635860	-4.0823860	-0.6669160
H	4.2169430	-4.1042930	1.0769760
H	3.6859130	-5.4412080	0.0483070
O	-0.3268820	1.6602180	-0.8473950
C	-0.2596200	2.9155790	-0.4478970
C	-1.2328000	3.8458030	-0.8890400
C	0.7462960	3.4002070	0.4216120
C	-1.1995920	5.1759790	-0.4799900
H	-2.0134630	3.4940760	-1.5607850
C	0.7698170	4.7343470	0.8234000
H	1.5129360	2.7048500	0.7595140
C	-0.2000610	5.6388530	0.3817120
H	-1.9652530	5.8617360	-0.8397100
H	1.5600600	5.0723260	1.4923130
I	-2.7904730	0.2191620	-0.2289970
C	-4.5672820	-0.8519130	0.2248120
C	-4.6078120	-2.2356190	0.0413580
C	-5.6870310	-0.1691240	0.7041040
C	-5.7782030	-2.9353740	0.3387000
H	-3.7368090	-2.7682560	-0.3299150
C	-6.8519530	-0.8791130	0.9988540
H	-5.6567940	0.9071420	0.8481480
C	-6.9015930	-2.2611660	0.8171930
H	-5.8068430	-4.0125790	0.1944090
H	-7.7222580	-0.3448090	1.3718500
H	-0.1770520	6.6783390	0.6992000
H	-7.8108670	-2.8099610	1.0476270

Complex E'(1)

Cu	0.2810990	0.0378300	0.0462740
O	-1.06956401	.5783820	0.2809900
C	-2.33418001	.5176870	0.2078490
C	-3.07479900	.4142310	-0.2549420
C	-3.06512202	.8000130	0.6704020
C	-2.5532910	-0.8070700	-0.7553120
O	-1.3321470	-1.1079090	-0.8143940
C	-3.5693730	-1.8588360	-1.2648090
C	1.4826780	-1.14123901	.2869060
C	2.5889520	-0.36792501	.7183640
C	0.2275100	-1.00491101	.9327140
C	2.4327940	0.5309890	2.7585780
H	3.5531110	-0.48660801	.2340570
C	0.1087660	-0.08547102	.9994060
H	-0.5805090	-1.70000301	.7242820
C	1.1923620	0.6721760	3.4070170
H	3.2841040	1.1273940	3.0766310
H	-0.84904400	.0043740	3.5053310
H	1.0895700	1.3698270	4.2337920
I	1.8931060	-2.89804100	.1341580
H	-4.15219700	.5124150	-0.2599840
C	-2.8351810	-3.0818780	-1.8161500
H	-2.2085840	-3.5535450	-1.0522010
H	-3.5666380	-3.8211560	-2.1659970
H	-2.1876010	-2.8152460	-2.6583900
C	-4.4678780	-2.3044860	-0.0999970
H	-5.0579560	-1.47510500	.3039870
H	-5.1660490	-3.0799090	-0.4413610
H	-3.8711980	-2.72624600	.7183890
C	-4.4364200	-1.2604910	-2.3834470
H	-3.8163200	-0.9041110	-3.2151510
H	-5.1182760	-2.0261610	-2.7757960
H	-5.0443830	-0.4202850	-2.0323360
C	-4.59084002	.7302260	0.5847420
H	-4.93801002	.5703550	-0.4428910
H	-5.00237101	.9339350	1.2163110
H	-5.01761803	.6795430	0.9321780
C	-2.66594503	.0683360	2.1292970
H	-1.57927503	.1513640	2.2268170
H	-3.11975704	.0043810	2.4790070
H	-3.00928402	.2605550	2.7884180
C	-2.57473003	.9601110	-0.2091090
H	-3.02021004	.9046400	0.1285260
H	-1.48543504	.0519070	-0.1600190
H	-2.86024903	.8079500	-1.2578210
O	1.4672260	0.5179070	-1.4979840
C	2.2719590	1.5447520	-1.5329020
C	2.2660570	2.5714790	-0.5486460
C	3.2144740	1.6945860	-2.5886750
C	3.1353570	3.6568120	-0.6202440
H	1.5527200	2.4904660	0.2700230
C	4.0780310	2.7846220	-2.6491160
H	3.2448140	0.9267730	-3.3605020
C	4.0537350	3.7820270	-1.6679770
H	3.0939480	4.4205200	0.1558420
H	4.7826100	2.8577830	-3.4768920
H	4.7299820	4.6318180	-1.7191490

TS'1 (1)

Negative frequency: -62,7 cm^{-1}

Cu	-0.6531430	0.1417300	-0.3756080
O	0.2855000	-0.5348630	1.4075160
C	1.4668210	-0.9823200	1.4979850
C	2.4068740	-1.0216020	0.4491100
C	1.8504260	-1.5141540	2.8986920
C	2.2208600	-0.5541480	-0.8741660
O	1.1699600	-0.0201570	-1.3237810
C	3.4041270	-0.7026010	-1.8596840
C	-2.6567100	-0.3018330	-0.0082680
C	-2.7926080	-0.4966240	1.3729630
C	-3.5397520	0.5314100	-0.7082150
C	-3.7703170	0.2182380	2.0627140
H	-2.1196790	-1.1660610	1.8977030
C	-4.5139630	1.2307600	-0.0004530
H	-3.4562080	0.6447410	-1.7843580
C	-4.6334860	1.0795430	1.3826820
H	-3.8600570	0.0906760	3.1389480
H	-5.1874150	1.8935980	-0.5386410
H	-5.4030820	1.6213290	1.9260070
I	-1.7868040	-2.0488750	-1.2273600
H	3.3764340	-1.4459450	0.6726930
C	3.0271700	-0.1359530	-3.2293660
H	2.7811080	0.9293200	-3.1690100
H	3.8717110	-0.2541610	-3.9197000
H	2.1613880	-0.6547770	-3.6539900
C	4.6263400	0.0631200	-1.3292920
H	4.9832860	-0.3375660	-0.3747200
H	5.4502810	-0.0060030	-2.0513180
H	4.3931570	1.1251430	-1.1849700
C	3.7575500	-2.1896330	-2.0207860
H	4.0946600	-2.6377380	-1.0801630
H	2.8937310	-2.7632340	-2.3790230
H	4.5653710	-2.3023750	-2.7553780
C	1.6809430	-0.3585330	3.8965150
H	0.6630330	0.0412940	3.8583010
H	1.8807960	-0.7085900	4.9172620
H	2.3798040	0.4587820	3.6769770
C	0.8686140	-2.6398660	3.2561070
H	-0.1646780	-2.2812940	3.2193590
H	0.9645660	-3.4834950	2.5606820
H	1.0714250	-3.0115560	4.2685470
C	3.2778920	-2.0531750	3.0085770
H	3.4492820	-2.9041680	2.3386990
H	4.0263750	-1.2832090	2.7869340
H	3.4566020	-2.4006310	4.0339360
O	-0.9589690	2.1248020	-0.5903310
C	-0.1191960	3.0702840	-0.2589050
C	-0.3466290	4.4123130	-0.6728010
C	1.0419510	2.8449270	0.5295350
C	0.5179580	5.4442840	-0.3193650
H	-1.2276370	4.6176170	-1.2792740
C	1.8992300	3.8863030	0.8757970
H	1.2483990	1.8289850	0.8582970
C	1.6541970	5.1990880	0.4593870
H	0.3020550	6.4571070	-0.6578900
H	2.7773680	3.6681200	1.4831350
H	2.3280240	6.0070610	0.7338370

Complex F' (1)

Cu	-0.6353570	-0.3458880	-0.5785570
O	0.2120980	0.5041970	1.2207900
C	1.4302030	0.4224700	1.5447680
C	2.4542550	-0.07437300	.7103930
C	1.7641750	0.9229690	2.9676310
C	2.2914260	-0.5296430	-0.6106830
O	1.1932940	-0.6118640	-1.2404030
C	3.5480000	-0.9793730	-1.3869500
I	-0.8980020	-2.83851700	.0812440
C	-2.4828820	-0.1801030	-0.1111380
C	-3.4712720	-0.4431230	-1.0525530
C	-2.78700900	.3189940	1.1469070
C	-4.8038940	-0.1844980	-0.7238330
H	-3.2191190	-0.8308600	-2.0357480
C	-4.12746400	.5768510	1.4636430
H	-1.99853400	.5136430	1.8681860
C	-5.13483600	.3252620	0.5342480
H	-5.5828820	-0.3824060	-1.4571850
H	-4.37495600	.9727090	2.4466150
H	-6.17375300	.5229300	0.7867490
H	3.4618800	-0.08199801	.1031600
C	3.1765120	-1.4182320	-2.8044080
H	2.7145390	-0.6029320	-3.3708560
H	4.0828140	-1.7340030	-3.3354500
H	2.4746620	-2.2583290	-2.7938660
C	4.5533520	0.1792840	-1.4750170
H	4.1134510	1.0458530	-1.9834440
H	4.8970980	0.5042700	-0.4877240
H	5.4327430	-0.1380740	-2.0497860
C	4.1913080	-2.1681750	-0.6543960
H	4.5423370	-1.89392400	.3457860
H	3.4807070	-2.9970320	-0.5494900
H	5.0540250	-2.5316180	-1.2269520
C	3.2430700	0.8194260	3.3443520
H	3.6014380	-0.21646003	.3213210
H	3.8791690	1.4205930	2.6840050
H	3.3829290	1.1936390	4.3661310
C	0.9404100	0.0863270	3.9585550
H	1.1098110	0.4429510	4.9822510
H	-0.12885800	.1609620	3.7380580
H	1.2264490	-0.97232203	.9169680
C	1.3289150	2.3930930	3.0600190
H	1.4917130	2.7695230	4.0776590
H	1.9065990	3.0212000	2.3702240
H	0.2681080	2.5003070	2.8149210
O	-0.97502601	.0638780	-1.8581670
C	-0.61766702	.3009140	-1.5415720
C	0.6844780	2.7768890	-1.8164850
C	-1.54348003	.2084290	-0.9772170
C	1.0341730	4.0989740	-1.5553040
H	1.4047260	2.0837500	-2.2437430
C	-1.18348604	.5275580	-0.7154400
H	-2.54572102	.8513730	-0.7525510
C	0.1062780	4.9854340	-1.0011830
H	2.0413280	4.4422650	-1.7848690
H	-1.91636005	.2074300	-0.2847660
H	0.3828060	6.0169120	-0.7971700

Complex C' (1)

	Cu	-0.2895140	0.0163560 -0.3983110
	O	0.9841900	1.2804080 0.0781970
	C	2.2464790	1.0597580 0.2329910
5	C	2.8790420	-0.1692920 0.0974140
	C	3.0211790	2.3314070 0.6037000
	C	2.2172680	-1.3757600 -0.2208840
	O	0.9717440	-1.4615990 -0.4336070
	C	3.0282480	-2.6733300 -0.3204240
10	H	3.9469570	-0.2098320 0.2565870
	C	2.1155080	-3.8515820 -0.6630970
	H	1.6090040	-3.7035600 -1.6222680
	H	2.7170900	-4.7653840 -0.7309720
	H	1.3482280	-4.0033610 0.1029940
15	C	4.0892470	-2.5183130 -1.4230460
	H	4.7996140	-1.7149170 -1.2030090
	H	4.6559570	-3.4527240 -1.5135920
	H	3.6243710	-2.3088630 -2.3934490
	C	3.7171600	-2.9438020 1.0277860
20	H	4.4259410	-2.1538770 1.2962920
	H	2.9828460	-3.0348470 1.8366280
	H	4.2731100	-3.8870930 0.9675050
	C	2.8160090	3.3566850 -0.5237160
	H	1.7546040	3.5788500 -0.6673780
25	H	3.3338640	4.2889610 -0.2695680
	H	3.2258170	2.9892650 -1.4723390
	C	2.4283880	2.8812390 1.9114700
	H	1.3620520	3.0982780 1.8005870
	H	2.5543560	2.1667750 2.7340370
30	H	2.9451080	3.8082810 2.1860470
	C	4.5198360	2.0939380 0.7966540
	H	4.7238960	1.3865700 1.6086410
	H	5.0000430	1.7260260 -0.1172970
	H	4.9982550	3.0441750 1.0603980
35	O	-1.6446340	-1.0812920 -0.9339950
	C	-2.6476280	-1.4526120 -0.1341660
	C	-3.8998070	-1.7259370 -0.7163930
	C	-2.4957640	-1.6390740 1.2521010
	C	-4.9548570	-2.1910430 0.0638240
40	H	-4.0193850	-1.5750740 -1.7863540
	C	-3.5632320	-2.0869960 2.0263700
	H	-1.5324000	-1.4303720 1.7143000
	C	-4.7986180	-2.3713060 1.4402460
	H	-5.9118290	-2.4045360 -0.4073340
45	H	-3.4253680	-2.2203930 3.0970830
	H	-5.6277790	-2.7245320 2.0473870
	C	-1.5818290	1.4079130 -0.4444260
	C	-2.0306780	1.8644730 -1.6736720
	C	-1.9818600	1.9664940 0.7593170
50	C	-2.9138280	2.9499780 -1.6924130
	H	-1.7203940	1.3953270 -2.6033450
	C	-2.8757090	3.0434770 0.7225560
	H	-1.6161590	1.5944780 1.7129200
	C	-3.3371460	3.5342300 -0.4984700
55	H	-3.2751720	3.3264130 -2.6465410
	H	-3.2019300	3.4965510 1.6557730
	H	-4.0296510	4.3716790 -0.5198200

TS2' (1)

Negative frequency: -305,3 cm^{-1}

Cu	-0.316449	00.112217	0 -0.433500
O	1.050665	0 1.319806	0 0.078875
C	2.286201	0 1.014027	0 0.249639
C	2.834016	0 -0.26194	900.100152
C	3.157480	0 2.212261	0 0.657463
C	2.124367	0 -1.431753	0 -0.260134
O	0.881160	0 -1.467748	0 -0.499380
C	2.896553	0 -2.756201	0 -0.373417
C	-1.826079	01.339194	0 -0.473593
C	-1.871450	02.178862	0 -1.581644
C	-2.393118	01.662424	0 0.751709
C	-2.445475	03.439665	0 -1.417063
H	-1.469434	01.868321	0 -2.541894
C	-2.963539	02.931879	0 0.888376
H	-2.385224	00.964414	0 1.584884
C	-2.989668	03.819320	0 -0.187123
H	-2.475240	04.121568	0 -2.263404
H	-3.391662	03.216784	0 1.846205
H	-3.444490	04.799282	0 -0.072973
H	3.895147	0 -0.37046	000.276630
C	1.950466	0 -3.893548	0 -0.761825
H	1.473096	0 -3.707647	0 -1.729429
H	2.518629	0 -4.828539	0 -0.834488
H	1.158979	0 -4.031140	0 -0.017830
C	3.986026	0 -2.621248	0 -1.450104
H	3.549872	0 -2.370497	0 -2.424366
H	4.722499	0 -1.851388	0 -1.197900
H	4.518235	0 -3.574822	0 -1.553331
C	3.546604	0 -3.086189	00.980561
H	4.278488	0 -2.330044	01.282728
H	2.792480	0 -3.166481	01.772507
H	4.067898	0 -4.048826	00.911303
C	3.022715	0 3.289254	0 -0.431134
H	1.977840	0 3.584212	0 -0.564889
H	3.600215	0 4.177000	0 -0.146536
H	3.407166	0 2.929556	0 -1.393508
C	2.607616	0 2.759088	0 1.985084
H	1.555691	0 3.042995	0 1.886508
H	2.691836	0 2.013418	0 2.785230
H	3.179985	0 3.644790	0 2.285976
C	4.637341	0 1.870450	0 0.836603
H	4.796913	0 1.131309	0 1.630226
H	5.087352	0 1.491361	0 -0.088383
H	5.182393	0 2.778624	0 1.119919
O	-1.998204	0-0.487178	0-1.017045
C	-2.813182	0-1.208126	0-0.207006
C	-4.167288	0-1.293254	0-0.559114
C	-2.346167	0-1.885496	00.925973
C	-5.034669	0-2.072066	00.202001
H	-4.517665	0-0.753493	0-1.434809
C	-3.225354	0-2.654247	01.687210
H	-1.294412	0-1.819391	01.971000
C	-4.570373	0-2.753710	01.329424
H	-6.081447	0-2.141177	00.083656
H	-2.853327	0-3.180333	02.562896
H	-5.251882	0-3.355069	01.924970

Complex D' (1)

Cu	0.1068480	-0.0322630	-0.0010760
O	-1.19761101	.4597870	0.0005800
C	-2.45553901	.2505110	0.0011210
C	-3.0728640	-0.01320700	.0006740
C	-3.30918502	.5345220	0.0021960
C	-2.4532250	-1.2849430	-0.0009880
O	-1.2024420	-1.4998840	-0.0021640
C	-3.3641900	-2.5304570	-0.0014160
H	-4.1543640	-0.02080000	.0014710
C	-2.5218300	-3.8074000	-0.0055070
H	-1.8772450	-3.86797500	.8775580
H	-3.1858300	-4.6802940	-0.0053830
H	-1.8814910	-3.8650360	-0.8918750
C	-4.2481710	-2.52482601	.2567200
H	-4.9187760	-1.65979101	.2867260
H	-4.8679060	-3.43017301	.2766370
H	-3.6379100	-2.51362702	.1678650
C	-4.2539330	-2.5207370	-1.2554160
H	-4.9254550	-1.6562270	-1.2792280
H	-3.6478910	-2.5056650	-2.1693170
H	-4.8730370	-3.4264970	-1.2758520
C	-2.93748303	.3428300	1.2553840
H	-1.86517303	.5594280	1.2770570
H	-3.48430804	.2938220	1.2627370
H	-3.19826602	.7960440	2.1702600
C	-2.93881903	.3438260	-1.2507740
H	-1.86653903	.5604820	-1.2733830
H	-3.20053302	.7977190	-2.1657900
H	-3.48569904	.2947960	-1.2568270
C	-4.81954302	.2920660	0.0028950
H	-5.14940601	.7427360	-0.8867580
H	-5.14848501	.7419180	0.8923850
H	-5.33879203	.2582060	0.0036040
O	2.1348330	0.0423260	-0.0008090
C	2.8014980	-1.18934100	.0004970
C	3.0981000	-1.7930220	-1.2152910
C	3.0997120	-1.78965701	.2175610
C	3.7149720	-3.0436830	-1.2066260
H	2.8448560	-1.2922750	-2.1454490
C	3.7166320	-3.04031301	.2115240
H	2.8477230	-1.28635002	.1466770
C	4.0243280	-3.66684000	.0031100
H	3.9505680	-3.5311400	-2.1486590
H	3.9534840	-3.52515202	.1545930
H	4.5029270	-4.64222700	.0041370
C	2.8832220	1.2178080	-0.0011880
C	4.2742520	1.2132550	-0.0020110
C	2.1596840	2.4075250	-0.0007730
C	4.9476900	2.4364450	-0.0024390
H	4.8300260	0.2813920	-0.0023360
C	2.8485820	3.6173220	-0.0012020
H	1.0714660	2.3786450	-0.0001320
C	4.2445310	3.6390730	-0.0020510
H	6.0344650	2.4383280	-0.0030900
H	2.2864750	4.5474560	-0.0008830
H	4.7777410	4.5855160	-0.0023930

Complex B'' (1)

Cu	-0.7534060	-1.2645780	-0.0854090
O	-3.0000220	-1.5056980	-0.0198350
C	-3.7766850	-0.5196410	0.0202120
C	-3.3564570	0.8381350	0.0155130
C	-2.0421940	1.3197900	-0.0258030
O	-0.9764690	0.6168620	-0.0671300
C	-1.8323570	2.8517660	-0.0230050
O	-0.1585020	-3.0176940	-0.1221170
H	-0.9745810	-3.5395430	-0.1028320
H	-4.1390450	1.5881730	0.0487360
C	-5.2992310	-0.7940580	0.0791060
C	-5.5641070	-2.2999600	0.0847050
H	-5.0962140	-2.7865340	0.9470490
H	-6.6448820	-2.4826740	0.1321780
H	-5.1750590	-2.7800360	-0.8194830
C	-5.9854510	-0.1742530	-1.1483260
H	-7.0597850	-0.3987400	-1.1282190
H	-5.8713830	0.9145050	-1.1783640
H	-5.5733310	-0.5834850	-2.0789060
C	-5.8875290	-0.1830040	1.3607330
H	-6.9588720	-0.4128950	1.4254190
H	-5.4003490	-0.5942620	2.2534090

H	-5.7772050	0.9061850	1.3871860
C	-0.3419930	3.1958400	-0.0596300
H	0.1421370	2.8020320	-0.9591440
H	-0.2222520	4.2864430	-0.0563850
H	0.1875710	2.7914120	0.8091430
C	-2.4429960	3.4586670	1.2506380
H	-3.5243140	3.2962600	1.3071920
H	-1.9878710	3.0266080	2.1501320
H	-2.2644950	4.5414610	1.2688390
C	-2.5083780	3.4683650	-1.2585870
H	-2.3301770	4.5512060	-1.2787450
H	-2.1021120	3.0422550	-2.1839850
H	-3.5913630	3.3065420	-1.2586070
I	2.3636760	-0.6501190	-0.0114550
C	4.4171700	-0.0601370	0.0300370
C	4.7472160	1.2947490	-0.0170320
C	5.4135670	-1.0341460	0.1024470
C	6.0905150	1.6737060	0.0078720
H	3.9694750	2.0512230	-0.0730570
C	6.7533760	-0.6430420	0.1268830
H	5.1542470	-2.0883980	0.1394810
C	7.0949780	0.7085200	0.0797520
H	6.3478780	2.7294160	-0.0292630
H	7.5298300	-1.4020350	0.1830300
H	8.1393890	1.0083980	0.0987240

References

[1] a) M. J. Frisch, *et al.* Gaussian 09, revision A.02; Gaussian, Inc ; Wallingford, CT, 2009; b) C. Adamo, V. J. Barone, *Chem. Phys.,* 1999, **110,** 6158; c) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett*., 1996, **77,** 3865; d) R. Krishnan, J. S. Binkley, R. Seeger, J. A. J. Pople, *Chem. Phys.,* 1980, ***72,*** 650; e) T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. V. R. J. Schleyer, *Comput. Chem.,* 1983, **4,** 294; f) L. v. Szentpaly, P. Fuentealba, H. Preuss, H. Stoll, *Chem. Phys. Lett.,* 1982, **93,** 555; g) W. Kuchle, M. Dolg, H. Stoll, H. Preuss, *J. Chem. Phys.,* 1994, **100,** 7535. h) J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.,* 2005, **105,** 2999.