

Supporting Information

**Intramolecular Interactions in a Heterometallic Copper(II)-Lead(II) Tetranuclear  $\beta$ -Diketonate Complex: Insights from Thermodynamics, Molecular Spectroscopies and Quantum Chemical Calculations**

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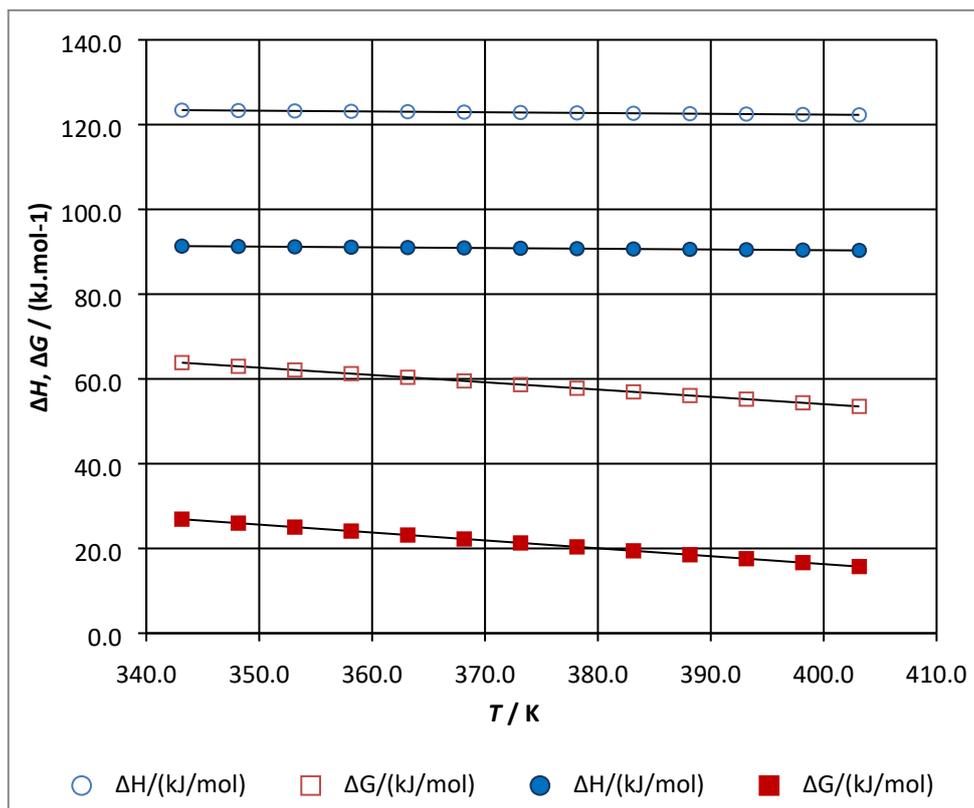
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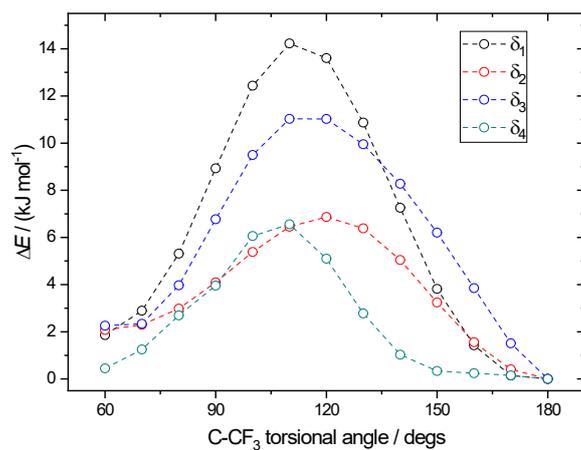
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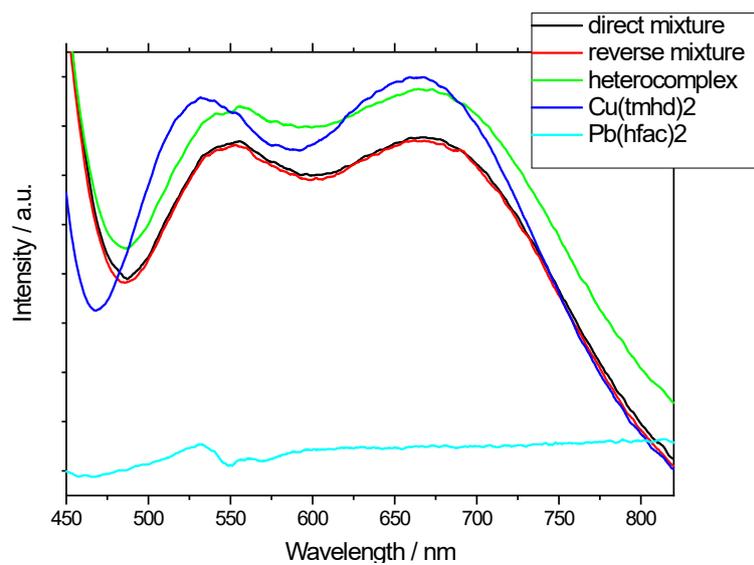




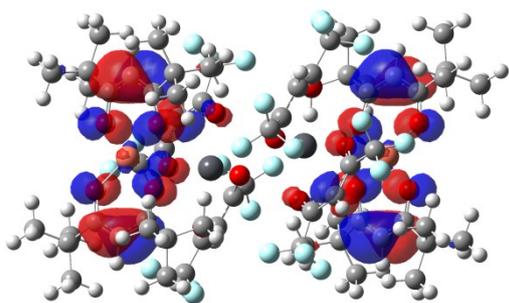
**Figure S1.** Changes in enthalpies (circles) and Gibbs free energy (squares) for reaction (10) as a function of the temperature. Unfilled and filled markers refer to BS1 and BS2, respectively.



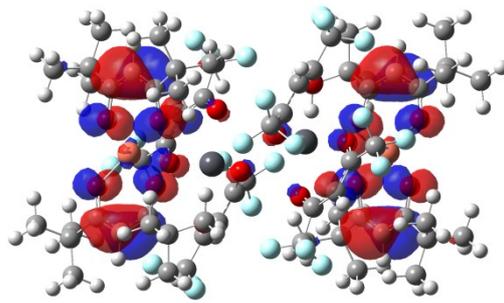
**Figure S2.** Potential energy surface of  $[\text{Cu}(\text{tmhd})_2\text{Pb}(\text{hfac})_2]$  scanned about the dihedral angles  $\delta_1 = (\text{O5}, \text{C16}, \text{C21}, \text{F90})$ ,  $\delta_2 = (\text{O4}, \text{C14}, \text{C16}, \text{F87})$ ,  $\delta_3 = (\text{O3}, \text{C11}, \text{C15}, \text{F83})$ , and  $\delta_4 = (\text{O6}, \text{C20}, \text{C22}, \text{F92})$ . (For the atoms' labelling, refer to the optimised geometries.)



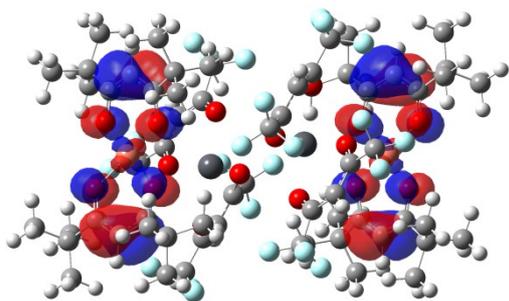
**Figure S3.** UV-Vis absorption spectra of the compounds in toluene solution: direct mixture =  $\text{Cu}(\text{tmhd})_2 + \text{Pb}(\text{hfac})_2$ , reverse mixture =  $\text{Cu}(\text{hfac})_2 + \text{Pb}(\text{tmhd})_2$ , heterocomplex =  $[\text{Cu}(\text{tmhd})_2 \text{Pb}(\text{hfac})_2]_2$ .



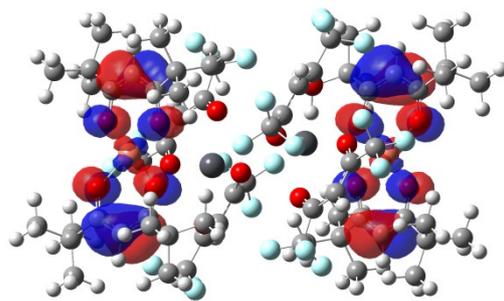
H-4  
(-0.24800)



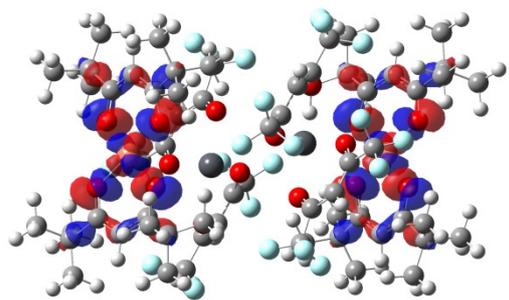
H-3  
(-0.24786)



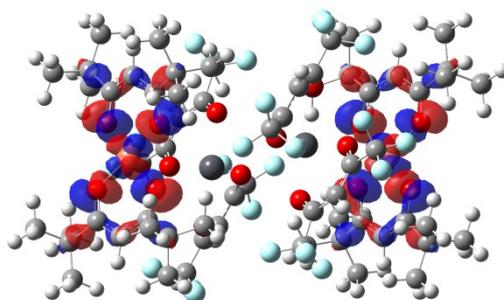
H-2  
(-0.23824)



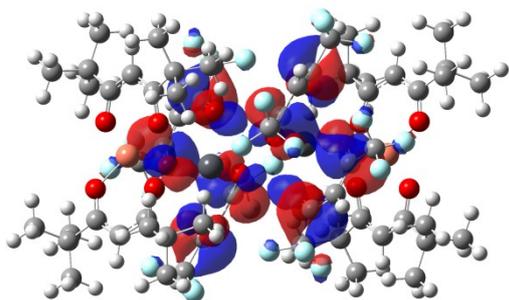
H-1  
(-0.23819)



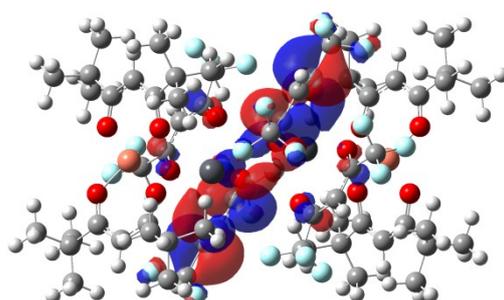
H  
(-0.17763)



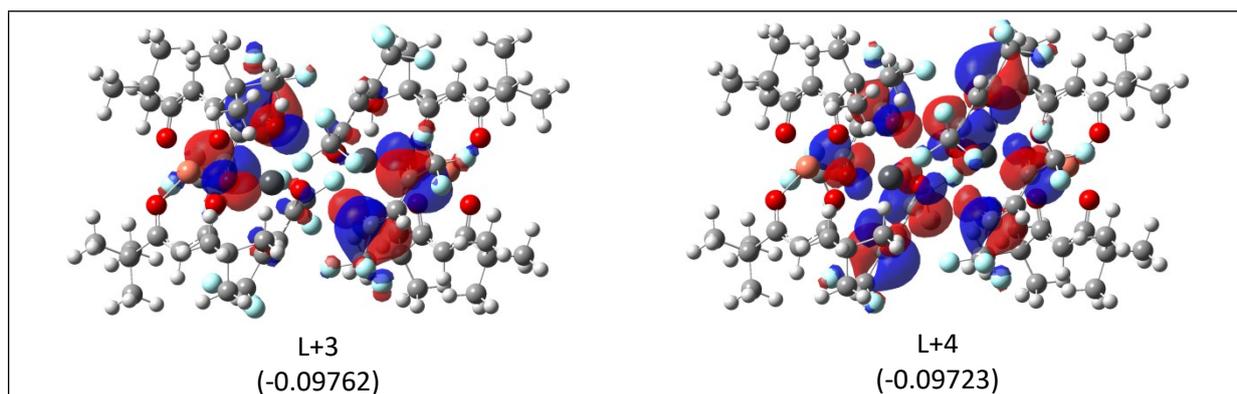
L  
(-0.16792)



L+1  
(-0.10146)



L+2  
(-0.09980)



**Figure S4.** Plot of frontier molecular orbitals (FMOs) of  $[\text{Cu}(\text{tmhd})_2 \cdot \text{Pb}(\text{hfac})_2]_2$ . Corresponding eigenvalues are also reported in units of hartree. Level of theory: UB3LYP[GD3BJ] / H : 3-21G ; C. O. Cu : 6-31+G(d); Pb : LANLD2Z.

## S2 Tables

**Table S1.** Comparison between calculated and experimental average values of selected interatomic distances along with their standard deviations (all values in units of  $10^{-10}$  m). T and S indicate the spin multiplicity (triplet and singlet, respectively), whereas BS1 and BS2 indicate the different basis set (see main text).

	comp. T(BS1)	comp. T(BS2)	comp. S(BS1)	comp. S(BS2)	crystal data
<Cu-O> std.dev.	1.935 0.013	1.934 0.016	1.951 0.016	1.950 0.016	1.912(19)
<Cu-O'(Pb)> std.dev.	2.499 0.000	2.540 0.005	2.509 0.000	2.574 0.005	2.558(4)
<Pb-O <sub>short</sub> > std.dev.	2.379 0.038	2.386 0.057	2.377 0.041	2.384 0.057	2.366(4)
<Pb-O <sub>long</sub> > std.dev.	2.442 0.008	2.458 0.008	2.447 0.029	2.458 0.016	2.551(4)
<Pb-O'(Cu)> std.dev.	2.839 0.098	2.807 0.095	2.829 0.067	2.805 0.085	2.761(4) ; 2.931(4)
<Pb-O'(Pb')> std.dev.	2.871 0.000	2.881 0.003	2.835 0.000	2.868 0.004	2.860(4) ; 2.430(4)
Pb...Cu	3.346	3.348	3.347	3.338	3.4169(6)
Pb...Pb	4.135	4.122	4.044	4.115	4.2355(3)

**Table S2.** Energy differences between LUMO and HOMO and between (LUMO+1) and HOMO of [Cu(tmhd)<sub>2</sub>Pb(hfac)<sub>2</sub>] (in units of eV).

Spin Multiplicity		$\Delta E(\text{HOMO-LUMO}) / \text{eV}$	$\Delta E(\text{HOMO-(LUMO+1)}) / \text{eV}$	
Singlet		0.268	2.120	#
		0.264	2.073	##
Triplet	$\alpha$	3.748	3.923	#
	$\beta$	3.671	3.758	
	$\alpha$	3.734	3.864	##
	$\beta$	3.658	3.726	

Level of theory: # B3LYP[GD3BJ] / H : 3-21G ; C : 6-31G(d); O, Cu : 6-31+G(d); Pb : LANLD2Z; ## B3LYP[GD3BJ] / H : 3-21G ; C, O, Cu : 6-31+G(d); Pb : LANLD2Z

**Table S3.** NBO analysis of [Cu(tmhd)<sub>2</sub>Pb(hfac)<sub>2</sub>]<sub>2</sub>. Data shown only for orbitals involving metals. Geometry optimised at DFT B3LYP[GD3BJ] / H : 3-21G ; C, O, Cu : 6-31+G(d); Pb : LANLD2Z. Level of Theory for NBO analysis: HF / H : 3-21G ; C, O, Cu : 6-31+G(d); Pb : LANLD2Z. Cutoff = 5.00 kcal/mol.

Donor				Acceptor				$\Delta E^{(2)}$ / (kcal/mol)
LP*	( 2 )	Pb	1	→	LP*	( 3 )	Pb 1	6.39
LP*	( 4 )	Pb	1	→	LP*	( 2 )	Pb 1	34.60
LP*	( 4 )	Pb	1	→	LP*	( 3 )	Pb 1	6.32
LP	( 1 )	Pb	1	→	LP*	( 6 )	Cu 2	15.30
LP*	( 3 )	Pb	1	→	LP*	( 6 )	Cu 2	5.73
LP*	( 4 )	Pb	1	→	LP*	( 5 )	Cu 2	66.54
LP*	( 2 )	Pb	1	→	LP*	( 3 )	Pb 95	24.62
LP*	( 3 )	Pb	1	→	LP*	( 2 )	Pb 95	83.27
LP*	( 3 )	Pb	1	→	LP*	( 3 )	Pb 95	18.47
LP*	( 3 )	Pb	1	→	LP*	( 4 )	Pb 95	13.00
BD	( 1 )	Cu	2 - O 8	→	LP*	( 2 )	Pb 1	8.46
BD	( 1 )	Cu	2 - O 8	→	LP*	( 3 )	Pb 1	7.34
CR	( 3 )	Cu	2	→	LP*	( 2 )	Pb 1	6.59
LP	( 1 )	O	8	→	LP*	( 3 )	Pb 1	9.45
BD	( 1 )	Cu	2 - O 7	→	RY*	( 1 )	C 23	7.53
BD	( 1 )	Cu	2 - O 7	→	BD*	( 1 )	Cu 2 - O 8	8.45
BD	( 1 )	Cu	2 - O 7	→	BD*	( 1 )	C 23 - C 27	10.70
BD	( 1 )	Cu	2 - O 8	→	RY*	( 1 )	C 26	6.86
BD	( 1 )	Cu	2 - O 8	→	BD*	( 1 )	Cu 2 - O 7	7.92
BD	( 1 )	Cu	2 - O 8	→	BD*	( 1 )	C 26 - C 40	10.70
BD	( 1 )	C	23 - C 27	→	BD*	( 1 )	Cu 2 - O 7	8.10
BD	( 1 )	C	26 - C 40	→	BD*	( 1 )	Cu 2 - O 8	7.64
LP	( 1 )	O	7	→	LP*	( 6 )	Cu 2	9.19
LP	( 1 )	O	8	→	LP*	( 6 )	Cu 2	7.57
BD*	( 1 )	Cu	2 - O 7	→	LP*	( 6 )	Cu 2	6.33
BD*	( 1 )	Cu	2 - O 8	→	LP*	( 6 )	Cu 2	8.58
BD*	( 1 )	Cu	2 - O 8	→	BD*	( 2 )	O 5 - C 17	8.29
BD	( 1 )	O	4 - C 14	→	LP*	( 3 )	Pb 1	7.50
LP	( 1 )	O	3	→	LP*	( 2 )	Pb 1	6.90
LP	( 1 )	O	3	→	LP*	( 4 )	Pb 1	17.60
LP	( 2 )	O	3	→	LP*	( 4 )	Pb 1	5.08
LP	( 1 )	O	4	→	LP*	( 3 )	Pb 1	15.21
LP	( 2 )	O	4	→	LP*	( 3 )	Pb 1	24.47
LP	( 1 )	O	4	→	LP*	( 2 )	Pb 95	13.08
BD	( 1 )	O	5 - C 17	→	LP*	( 2 )	Pb 1	8.11
BD	( 1 )	O	6 - C 20	→	LP*	( 4 )	Pb 1	7.98
LP	( 1 )	O	5	→	LP*	( 2 )	Pb 1	14.93
LP	( 2 )	O	5	→	LP*	( 2 )	Pb 1	22.06
LP	( 1 )	O	6	→	LP*	( 4 )	Pb 1	22.59
LP	( 2 )	O	6	→	LP*	( 4 )	Pb 1	13.41
LP	( 1 )	O	5	→	LP*	( 7 )	Cu 2	7.91
LP	( 2 )	O	5	→	LP*	( 7 )	Cu 2	5.28
LP	( 1 )	O	10	→	LP*	( 3 )	Pb 1	8.85
BD	( 1 )	O	9 - C 53	→	LP*	( 5 )	Cu 2	7.06
BD	( 1 )	C	53 - C 57	→	LP*	( 5 )	Cu 2	5.28
LP	( 1 )	O	9	→	LP*	( 5 )	Cu 2	14.44
LP	( 1 )	O	9	→	LP*	( 6 )	Cu 2	7.36
LP	( 2 )	O	9	→	LP*	( 5 )	Cu 2	41.46
LP	( 2 )	O	9	→	LP*	( 6 )	Cu 2	7.35
LP	( 2 )	O	9	→	BD*	( 1 )	Cu 2 - O 8	57.40
LP	( 1 )	O	10	→	LP*	( 5 )	Cu 2	6.28
LP	( 1 )	O	10	→	LP*	( 6 )	Cu 2	11.88
LP	( 2 )	O	10	→	LP*	( 5 )	Cu 2	25.93
LP	( 2 )	O	10	→	LP*	( 6 )	Cu 2	18.97
LP	( 2 )	O	10	→	BD*	( 1 )	Cu 2 - O 7	54.36
LP*	( 2 )	Pb	95	→	LP*	( 3 )	Pb 95	6.90
LP*	( 2 )	Pb	95	→	LP*	( 4 )	Pb 95	48.51

LP	( 1 )	Pb	95			→	LP*	( 7 )	Cu	96			18.90
LP*	( 2 )	Pb	95			→	LP*	( 6 )	Cu	96			12.62
CR	( 3 )	Cu	96			→	LP*	( 2 )	Pb	95			7.81
LP	( 1 )	O	98			→	LP*	( 2 )	Pb	1			17.04
BD	( 1 )	O	98	- C	108	→	LP*	( 3 )	Pb	95			7.35
LP	( 1 )	O	97			→	LP*	( 4 )	Pb	95			19.49
LP	( 1 )	O	98			→	LP*	( 3 )	Pb	95			26.77
BD	( 1 )	O	99	- C	111	→	LP*	( 2 )	Pb	95			8.52
BD	( 1 )	O	100	- C	114	→	LP*	( 4 )	Pb	95			7.98
LP	( 1 )	O	99			→	LP*	( 2 )	Pb	95			18.04
LP	( 2 )	O	99			→	LP*	( 2 )	Pb	95			21.38
LP	( 1 )	O	100			→	LP*	( 4 )	Pb	95			25.43
LP	( 2 )	O	100			→	LP*	( 4 )	Pb	95			10.40
BD	( 1 )	C	111	- C	115	→	LP*	( 9 )	Cu	96			5.07
LP	( 1 )	O	99			→	LP*	( 9 )	Cu	96			5.40
LP	( 1 )	F	183			→	LP*	( 9 )	Cu	96			5.49
LP	( 2 )	O	102			→	LP*	( 2 )	Pb	95			9.51
LP	( 2 )	O	102			→	LP*	( 3 )	Pb	95			8.82
LP	( 1 )	O	101			→	LP*	( 6 )	Cu	96			11.14
LP	( 2 )	O	101			→	LP*	( 6 )	Cu	96			31.15
LP	( 2 )	O	102			→	LP*	( 6 )	Cu	96			27.86
LP	( 2 )	O	102			→	LP*	( 7 )	Cu	96			7.06
LP	( 1 )	O	104			→	LP*	( 3 )	Pb	95			5.87
LP	( 2 )	O	104			→	LP*	( 2 )	Pb	95			5.99
LP	( 2 )	O	104			→	LP*	( 3 )	Pb	95			9.02
LP	( 1 )	O	103			→	LP*	( 6 )	Cu	96			10.96
LP	( 1 )	O	103			→	LP*	( 7 )	Cu	96			5.24
LP	( 2 )	O	103			→	LP*	( 6 )	Cu	96			28.62
LP	( 2 )	O	104			→	LP*	( 6 )	Cu	96			29.08
LP	( 2 )	O	104			→	LP*	( 7 )	Cu	96			5.13
LP	( 2 )	O	104			→	LP*	( 8 )	Cu	96			5.31
CR	( 3 )	Cu	2			→	BD*	( 1 )	Pb	1	- O	3	3.57
LP*	( 7 )	Cu	2			→	BD*	( 1 )	Pb	1	- O	3	10.32
LP	( 2 )	O	5			→	BD*	( 1 )	Pb	1	- O	3	13.47
LP	( 1 )	O	98			→	BD*	( 1 )	Pb	1	- O	3	5.68

**Table S4.** Orbitals' composition for [Cu(tmhd)<sub>2</sub>Pb(hfac)<sub>2</sub>]<sub>2</sub>.

Orbital						Occup.	%	%s	%p	%d	%f
BD	( 1 )	Cu	2	- O	7	1.94703					
							Cu	13.99	40.47	9.93	49.56
							O	86.01	12.92	86.93	0.15
BD	( 1 )	Cu	2	- O	8	1.94315					
							Cu	12.95	40.10	10.45	49.40
							O	87.05	14.75	85.17	0.07
BD	( 1 )	O	4	- C	14	1.99234					
							O	65.67	40.31	59.59	0.10
							C	34.33	30.38	69.33	0.29
BD	( 1 )	O	5	- C	17	1.99156					
							O	66.08	41.28	58.62	0.10
							C	33.92	29.80	69.89	0.30
BD	( 1 )	O	6	- C	20	1.99253					
							O	65.58	40.95	58.67	0.38
							C	34.42	31.00	68.84	0.16
BD	( 1 )	O	9	- C	53	1.99191					
							O	68.28	46.13	53.54	0.33
							C	31.72	26.62	73.16	0.21
BD	( 1 )	C	23	- C	27	1.95395					
							C	51.03	34.86	65.03	0.11
							C	48.97	22.54	77.31	0.15
BD	( 1 )	C	26	- C	40	1.95384					
							C	51.11	35.13	64.76	0.11
							C	48.89	22.69	77.16	0.15
BD	( 1 )	C	53	- C	57	1.95510					
							C	50.89	34.85	65.04	0.11
							C	49.11	22.59	77.26	0.15
BD	( 1 )	O	98	- C	##	1.99217					
							O	65.48	40.25	59.65	0.10
							C	34.52	30.45	69.25	0.29
BD	( 1 )	O	99	- C	##	1.99078					
							O	65.66	40.13	59.77	0.10
							C	34.34	30.13	69.58	0.29
BD	( 1 )	O	100	- C	##	1.99248					
							O	65.57	41.34	58.29	0.37
							C	34.43	31.04	68.80	0.16
BD	( 1 )	C	111	- C	##	1.97298					
							C	48.88	27.91	71.89	0.20
							C	51.12	33.21	66.59	0.20
CR	( 3 )	Cu	2			1.99715					
								100.00	0.00	0.00	1.00
CR	( 3 )	Cu	96			1.99685					
								100.00	0.00	0.00	1.00
LP	( 1 )	Pb	1			1.94005					
								98.11	1.89	0.00	1.00
LP	( 1 )	O	3			1.94696					
								53.02	46.90	0.08	10.00
LP	( 2 )	O	3			1.91747					
								5.37	94.49	0.14	90.00
LP	( 1 )	O	4			1.93646					
								38.88	61.08	0.04	90.00
LP	( 2 )	O	4			1.91894					
								20.86	79.10	0.04	20.00
LP	( 1 )	O	5			1.93957					
								34.42	65.53	0.05	20.00
LP	( 2 )	O	5			1.92158					
								24.28	75.69	0.03	10.00
LP	( 1 )	O	6			1.94939					
								52.93	46.99	0.08	10.00
LP	( 2 )	O	6			1.91883					
								6.07	93.79	0.14	20.00
LP	( 1 )	O	7			1.95430					
								42.15	57.74	0.11	20.00
LP	( 1 )	O	8			1.94440					
								41.14	58.82	0.04	20.00
LP	( 1 )	O	9			1.95538					
								42.00	57.90	0.11	20.00
LP	( 2 )	O	9			1.72442					
								11.82	88.03	0.15	30.00
LP	( 1 )	O	10			1.94551					
								40.24	59.72	0.04	30.00
LP	( 2 )	O	10			1.72446					
								13.53	86.40	0.07	50.00
LP	( 1 )	Pb	95			1.93278					
								97.78	2.22	0.00	10.00
LP	( 1 )	O	97			1.94850					
								55.34	44.58	0.08	90.00
LP	( 1 )	O	98			1.93033					
								58.69	41.30	0.02	0.00

LP	( 1 )	O	99		1.94356		43.39	56.56	0.05	0.00
LP	( 2 )	O	99		1.91462		16.46	83.50	0.04	80.00
LP	( 1 )	O	100		1.94650		53.72	46.21	0.07	90.00
LP	( 2 )	O	100		1.91780		4.88	94.98	0.14	0.00
LP	( 1 )	O	101		1.94851		39.14	60.74	0.12	0.00
LP	( 2 )	O	101		1.91734		20.68	79.24	0.09	40.00
LP	( 2 )	O	102		1.91676		51.03	48.95	0.02	20.00
LP	( 1 )	O	103		1.94902		40.33	59.56	0.11	20.00
LP	( 2 )	O	103		1.91970		19.40	80.51	0.09	10.00
LP	( 1 )	O	104		1.93789		13.65	86.30	0.05	10.00
LP	( 2 )	O	104		1.91693		46.51	53.48	0.02	80.00
LP	( 1 )	F	183		1.98254		71.36	28.62	0.02	80.00
BD*	( 1 )	Cu	2	- O 7	0.25535					
		Cu				86.01	40.47	9.93	49.56	0.05
		O				13.99	12.92	86.93	0.15	90.00
BD*	( 1 )	Cu	2	- O 8	0.26580					
		Cu				87.05	40.10	10.45	49.40	0.05
		O				12.95	14.75	85.17	0.07	10.00
LP*	( 2 )	Pb	1		0.12322		0.56	99.44	0.00	30.80
LP*	( 3 )	Pb	1		0.12071		0.87	99.13	0.00	30.80
LP*	( 4 )	Pb	1		0.10676		0.17	99.83	0.00	50.00
LP*	( 2 )	Pb	95		0.12484		1.26	98.74	0.00	10.00
LP*	( 7 )	Cu	2		0.04254		0.41	99.98	0.07	0.03
BD*	( 1 )	Pb	1	- O 3	0.05681					
		Pb				99.76	1.53	98.47		
		O				0.24	0.07	99.62	0.31	

**Table S5.** Values of NPA Charges (in units of  $e$ ) for  $\text{Cu}(\text{tmhd})_2$ ,  $\text{Pb}(\text{hfac})_2$ , and  $[\text{Cu}(\text{tmhd})_2\text{Pb}(\text{hfac})_2]_2$ .

		level of theory				
		#	##	###	####	#####
$\text{Cu}(\text{tmhd})_2$	Cu	1.46240	1.45276	1.42921	1.41328	1.41611
	O	-0.86933	-0.86428	-0.85352	-0.85589	-0.86234
$\text{Cu}(\text{hfa})_2$	Cu	1.47584	1.46862	1.44092	1.42745	1.42900
	O	-0.81881	-0.80970	-0.79450	-0.78917	-0.79821
$[\text{Cu}(\text{tmhd})_2\text{Pb}(\text{hfa})_2]_2$	Cu	1.24290	1.71781			
	O	-0.81958	-0.82728			
		-0.87934	-0.87848			
		-0.82795	-0.93289			
		-0.86525	-0.77276			

# UB3LYP[GD3BJ] / H : 3-21G ; C : 6-31G(d); O. Cu : 6-31+G(d); ## UB3LYP[GD3BJ] / H : 3-21G ; C. O. Cu : 6-31+G(d); ### UB3LYP[GD3BJ] / 6-31+G(d); #### UB3LYP[GD3BJ] / 6-311++G(d,p); ##### UB3LYP[GD3BJ] / 6-311++G(2df,p).

		level of theory				
		#	##	###	####	#####
$\text{Pb}(\text{tmhd})_2$	Pb	1.68084	1.67481	1.67493	1.67531	1.67531
	O	-0.90250	-0.89968	-0.89942	-0.89032	-0.89032
		-0.93792	-0.93806	-0.93793	-0.93304	-0.93304
$\text{Pb}(\text{hfac})_2$	Pb	1.71683	1.71112	1.71116	1.71597	1.71397
	O	-0.83911	-0.82883	-0.82877	-0.81121	-0.81321
		-0.89644	-0.88841	-0.88841	-0.87752	-0.88077
$[\text{Cu}(\text{tmhd})_2\text{Pb}(\text{hfac})_2]_2$	Pb	1.71726	1.69644			
	O	-0.80752	-0.80038			
		-0.88704	-0.85065			
		-0.89962	-0.81141			
		-0.81129	-0.84980			

# B3LYP[GD3BJ] / H : 3-21G ; C : 6-31G(d); O : 6-31+G(d); ## B3LYP[GD3BJ] / H : 3-21G ; C, O : 6-31+G(d); ### B3LYP[GD3BJ] / 6-31+G(d); #### B3LYP[GD3BJ] / 6-311++G(d,p); ##### B3LYP[GD3BJ] / 6-311++G(2d,2p). Pb : Always LANL2DZ.

**Table S6.** Mass spectrum of  $[\text{Cu}(\text{tmhd})_2\text{Pb}(\text{hfac})_2]_2$  (electron ionisation = 70 eV; evaporator temperature = 122 °C).

<b>m/z</b>	<b>Relative intensity (%)</b>	<b>Peak assignment</b>
63	42	$[\text{}^{63}\text{Cu}]^+$
189	100	$[\text{}^{63}\text{Cu}(\text{tmhd} - \text{C}_4\text{H}_9)]^+$
201	21	$[\text{Cu}(\text{hfac} - \text{CF}_3)]^+$
208	12	$[\text{}^{208}\text{Pb}]^+$
227	13	$[\text{PbF}]^+$
245	46	$[\text{Cu}(\text{tmhd} - \text{H})]^+$
315	22	$[\text{Cu}(\text{tmhd} - \text{C}_4\text{H}_9 - \text{C}_4\text{H}_8)]^+$
372	17	$[\text{Cu}(\text{tmhd})_2 - \text{C}_4\text{H}_9]^+$
391	16	$[\text{Pb}(\text{tmhd})]^+$
396	67	$[\text{Cu}(\text{hfac})(\text{tmhd} - \text{C}_4\text{H}_9)]^+$
415	26	$[\text{Pb}(\text{hfac})]^+$
453	49	$[\text{Cu}(\text{hfac})(\text{tmhd})]^+$
541	12	$[\text{Pb}(\text{hfac})\text{Cu}(\text{tmhd} - \text{C}_4\text{H}_9)]^+$
622	<5	$[\text{Pb}(\text{hfac})_2]^+$
754	42	$[\text{Pb}(\text{hfac})_2\text{Cu}(\text{tmhd} - 2\text{C}_4\text{H}_9)]^+$
775	35	$[\text{Cu}(\text{tmhd})_2\text{Pb}(\text{hfac} - \text{CF}_3)]^+$

**Table S7.** Comparison between experimental and computed wavenumbers and relative intensity ( $I^{\text{IR}}/I^{\text{IR}}_{\text{max}} \times 100$ ) for the 1.

Exp		T#		T##		S#		S##	
$\tilde{\nu}/\text{cm}^{-1}$	$I/I_{\text{max}} \times 100$								
3136	36	3174	4	3174	4	3187	2	3174	2
-	62	3164	3	3146	4	3165sh	2	3146	3
-	-	-	-	-	-	3156	3	-	-
2967	49	3143sh	3	3124sh	7	3141sh	5	-	-
2930sh	47	3121	21	3116sh	9	3134sh	7	3122sh	6
2910sh	-	3112	18	3099	26	3124	15	3116sh	6
-	-	-	-	-	-	3111	10	3099	15
2873	44	3057	11	3059	6	3061	13	3058sh	4
-	-	3051	10	3045	16	3053	11	3045	17
-	-	3046sh	9	3037	17	3045sh	8	3037	16
1732	1	1713	44	1710	44	1714	34	1709	31
1650	73	1700	30	1698	32	1702	21	1698	20
1604	49	1609	100	1616sh	15	1601	100	1593	100
-	-	1598sh	41	1603	95	-	-	-	-
1553	96	1570	73	1590	50	-	-	1547	24
-	-	1543	27	1564	74	1553	24	1536sh	11
1535	85	1538	26	1538	25	1544	16	1529sh	8
-	-	1520sh	7	1530sh	16	1531sh	8	-	-
-	-	1512sh	5	1521sh	10	1519sh	5	1520	6
1504	83	-	-	1512	8	-	-	1511	6
1462	70	1461	38	1455	43	1463	18	1454	20
-	-	1452sh	24	1445	21	1453	15	1444	12
-	-	1439	7	1431	6	1441	4	1432	3
1394	70	1422	11	1413	12	1421	7	1414	7
1362	63	1361	3	-	-	1366	2	-	-
1336sh	31	-	-	1340	2	1359	2	1341	2
1319	30	1322	4	1315	4	1307	7	-	-
-	-	1282	63	1283sh	9	1284	33	1297	7
1257	95	1267sh	14	1270	51	1268	10	1269	24
-	-	1241	78	-	-	1259	13	-	-
-	-	1229	40	1228	8	1240	51	-	-
1212	86	1217sh	15	-	-	1224sh	14	1227	5
1197sh	84	1183	57	1198	100	-	-	1198	55
-	-	1174	72	1179	30	1179	34	1176	29
1147	100	-	-	1143sh	35	1163sh	14	1150sh	6
-	-	1117	5	1132	71	1119	5	1140sh	9
-	-	-	-	-	-	-	-	1127	16
1083	55	1109	7	1099	7	1107	4	1099	5
1023	21	1056	1	1054	1	1059	1	1052	1
959	21	981	1	979	1	980	2	978	3
-	-	962	1	955	2	961sh	1	-	-
937	18	951	2	946	1	955	1	956	1
-	-	-	-	-	-	950	1	946	1
873	35	892	9	890	7	887	5	884	3
824sh	16	826	10	829	12	833sh	2	829	3
-	-	820sh	8	822sh	9	830sh	2	816	2
801	52	-	-	808sh	3	819	4	808sh	2
765	23	785	3	779	1	782	2	778	1
744	24	757	1	755	1	756	1	753	1
-	-	735	2	729	1	735	2	728	1
663	53	663	10	658	10	663	6	658	5
636	29	634	4	635	4	629	6	627	8
-	-	625sh	1	623sh	1	622	6	-	-
-	-	-	-	-	-	611	7	610	6
581	42	581	4	593sh	1	581	2	-	-
526	28	521	3	574	4	520	1	575	2
-	-	-	-	563sh	1	-	-	563sh	1
512	27	512	4	514	4	-	-	517sh	1
-	-	-	-	-	-	506sh	4	507sh	3
-	-	500	2	500	3	501	5	501	5
495	33	-	-	-	-	491	6	493	6
452	22	452	1	447	1	447	1	458	1
435sh	15	431	1	430	1	431sh	2	444	1
-	-	-	-	-	-	-	-	428sh	1
420	9	415	1	413	1	418	10	415	9
396	12	396	1	395	1	396sh	1	394sh	1
-	-	371sh	1	-	-	-	-	381	1
363	19	365	1	359	1	369	1	359	1
-	-	356	1	347	1	347	1	345	1

330	22	327	1	326	1	334	1	-	-
-	-	323	1	318	1	326	1	327	1
-	-	-	-	-	-	319	1	315	1
309	23	310	1	309	1	304	1	307	1
-	-	301	1	291	1	291	1	-	-
-	-	289	1	-	-	-	-	285	1
273	26	273	2	274	2	-	-	-	-
-	-	260sh	1	258sh	1	262	2	262	1
247sh	19	249	1	246	1	253sh	1	255sh	1
-	-	-	-	-	-	-	-	249sh	1
-	-	233	1	232	1	234	1	230	1
-	-	227	1	-	-	216	1	222sh	1
208	27	202	2	205	2	204sh	1	-	-
178	19	-	-	194sh	1	193	1	192	1
-	-	165	6	158	5	167	2	167	3
-	-	-	-	-	-	161sh	2	152	1
152	34	150sh	2	142	2	147	1	146sh	1
136	35	130	1	131sh	1	128	1	139sh	1
125sh	31	108	1	-	-	117	1	125	1
-	-	-	-	-	-	-	-	112sh	1
93	28	91	2	98	2	105	1	100	1
-	-	-	-	84	1	84	1	85	1
-	-	72	1	57	1	73	1	78sh	1
-	-	59	1	-	-	66	1	70sh	1
-	-	41	1	-	-	47	1	59	1
-	-	32	1	-	-	37	1	48	1
-	-	24	1	-	-	-	-	41sh	1

**Table S8.** Assignment of computed vibrational normal modes ( $1000\text{--}0\text{ cm}^{-1}$ ) for **1**, based on PED% (threshold  $\geq 3\%$ ), computed for the lowest triplet state. Level of theory: DFT B3LYP-D3(BJ) / BS1. Atoms coordinated by Cu are underlined; atoms coordinated by Pb are not underlined. Only modes with a PED contribution of  $\geq 3\%$  for **1** ( $\geq 10\%$  for precursors) are shown, with rare exceptions for specific Me–O or H–F interactions (marked by asterisks).

<b>1</b>				<b>Cu(tmhd)<sub>2</sub></b>			<b>Pb(hfac)<sub>2</sub></b>		
NM#	WN/c m <sup>-1</sup>	Int	Assignment	WN/c m <sup>-1</sup>	Int	Assignment	WN/ cm <sup>-1</sup>	Int	Assignment
28	54	3	$\nu_{\text{HF}}$ (3.2); $\chi_{\text{FC}\beta\text{FH}}$ (5.5); $\chi_{\text{HCHF/CHF}}$ (4.0); $\chi_{\text{CH/HCF}\beta}$ (3.8)						
35	60	5	$\nu_{\text{HF}}$ (4.0); $\chi_{\text{FC}\beta\text{FH}}$ (8.3); $\chi_{\text{CH/HCF}\beta}$ (6.0); $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{F}}$ (4.0); $\chi_{\text{C}\alpha\text{C}\beta\text{FH}}$ (4.0); $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}$ (3.9)						
38	65	4	$\nu_{\text{HF}}$ (3.4); $\chi_{\text{FC}\beta\text{FH}}$ (3.8); $\chi_{\text{HCHF/CHF}}$ (3.7); $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{F}}$ (3.0)						
41	71	3	$\nu_{\text{HF}}$ (4.5); $\chi_{\text{CH/HCF}\beta}$ (4.0); $\chi_{\text{OC}\alpha\text{C}\beta\text{C}}$ (3.5); $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{C}}$ (3.5); $\chi_{\text{FC}\beta\text{FH}}$ (3.5); $\chi_{\text{HCHF/CHF}}$ (3.0)						
43	73	2	$\nu_{\text{HF}}$ (4.5); $\chi_{\text{HCHF/CHF}}$ (7.1); $\chi_{\text{OC}\alpha\text{C}\beta\text{C}}$ (4.1); $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{C}}$ (3.2); $\chi_{\text{HCHO}}$ (3.2);						
46	80	4	$\nu_{\text{HF}}$ (5.1); $\nu_{\text{PbO}}$ (3.3); $\chi_{\text{HCHF/CHF}}$ (4.5)						
49	86	6	$\chi_{\text{OC}\alpha\text{C}\gamma\text{C}\alpha}$ (12.0); $\chi_{\text{HCHF/CHF}}$ (5.0); $\chi_{\text{CuOC}\alpha\text{C}\beta}$ (3.5); $\chi_{\text{CuOC}\alpha\text{C}\gamma}$ (3.3)						
51	89	15	$\nu_{\text{HF}}$ (4.4); $\chi_{\text{OCuOC}\alpha}$ (3.8)						
54	93	15	$\nu_{\text{HF}}$ (5.7); $\nu_{\text{PbO}}$ (3.3); $\chi_{\text{FC}\beta\text{FH}}$ (7.6); $\chi_{\text{C}\alpha\text{C}\beta\text{FH}}$ (6.5); $\chi_{\text{CH/HCF}\beta}$ (6.1); $\chi_{\text{HCHF/CHF}}$ (5.7)				90	4	$\nu_{\text{PbO}}$ (8.7); $\chi_{\text{OPbOC}\alpha}$ (15.3); $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{F}}$ (13.6); $\chi_{\text{C}\alpha\text{C}\gamma\text{C}\alpha\text{C}\beta}$ (11.0)
55	97	8	$\nu_{\text{HF}}$ (3.9); $\chi_{\text{HCHF/CHF}}$ (5.0); $\chi_{\text{FC}\beta\text{FH}}$ (4.8); $\chi_{\text{C}\alpha\text{C}\gamma\text{C}\alpha\text{C}\beta}$ (4.4); $\chi_{\text{OC}\alpha\text{C}\gamma\text{C}\alpha}$ (3.2)				99	2	$\chi_{\text{OC}\alpha\text{C}\beta\text{F}}$ (23.0); $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{F}}$ (12.2); $\chi_{\text{OPbOC}\alpha}$ (9.7); $\chi_{\text{C}\alpha\text{C}\gamma\text{C}\alpha\text{C}\beta}$ (9.6)
58	103	7	$\nu_{\text{HF}}$ (3.0); $\chi_{\text{FC}\beta\text{FH}}$ (5.6); $\chi_{\text{CH/HCF}\beta}$ (4.6); $\chi_{\text{C}\alpha\text{C}\beta\text{FH}}$ (3.2)				100	3	$\chi_{\text{OC}\alpha\text{C}\beta\text{F}}$ (14.2), $\chi_{\text{C}\gamma\text{C}\alpha\text{C}\beta\text{F}}$ (9.6)
60	107	6	$\nu_{\text{HF}}$ (3.2); $\chi_{\text{FC}\beta\text{FH}}$ (8.3); $\chi_{\text{CH/HCF}\beta}$ (4.3); $\chi_{\text{C}\alpha\text{C}\beta\text{FH}}$ (4.1)						
63	110	7	$\nu_{\text{HF}}$ (3.8); $\chi_{\text{FC}\beta\text{FH}}$ (4.7); $\chi_{\text{HCHF/CHF}}$ (3.9); $\chi_{\text{CH/HCF}\beta}$ (3.5)						

66	117	2	$\chi_{\text{OCuOC}\alpha}(5.6)$ ; $\chi_{\text{OC}\alpha\text{C}\beta\text{C}}(5.6)$ ; $\chi_{\text{CaCyCaC}\beta}(3.4)$				
70	130	7	$\chi_{\text{FC}\beta\text{FH}}(4.4)$				
72	131	5	$\chi_{\text{FC}\beta\text{FH}}(3.2)$				
76	142	6	$\nu_{\text{OH}}(3.2)$ ; $\chi_{\text{FC}\beta\text{FH}}(5.8)$ ; $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}(4.8)$ ; $\chi_{\text{OPbOC}\alpha}(3.6)$ ; $\chi_{\text{CH}/\text{HCFC}\beta}(3.6)$ ; $\chi_{\text{HCHF}/\text{CHF}}(3.0)$			138 12 $\chi_{\text{CyCaC}\beta\text{F}}(19.8)$ ; $\chi_{\text{OPbOC}\alpha}(14.8)$	
77	148	6	$\chi_{\text{OCuOC}\alpha}(3.1)$				
80	150	21	$\chi_{\text{HCHF}/\text{CHF}}(3.7)$				
82	159	9	$\nu_{\text{OH}}(3.8)$ ; $\chi_{\text{OCuOC}\alpha}(7.6)$				
83	165	113	$\nu_{\text{CuO}}(2.8)^*$ ; $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}(9.1)$ ; $\chi_{\text{OPbOC}\alpha}(8.6)$ ; $\chi_{\text{CyCaC}\beta\text{F}}(6.0)$ ; $\chi_{\text{C}\beta\text{CaCyCa}}(3.0)$			161 40 $\nu_{\text{PbO}}(7.0)^*$ ; $\chi_{\text{OPbOC}\alpha}(19.6)$ ; $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}(16.6)$ ; $\chi_{\text{CyCaC}\beta\text{F}}(14.4)$	
88	202	30	$\chi_{\text{OCuOC}\alpha}(5.0)$				
90	205	14	$\chi_{\text{OPbOC}\alpha}(5.7)$ ; $\chi_{\text{CyCaC}\beta\text{F}}(3.1)$ ; $\chi_{\text{OCuOC}\alpha}(3.1)$	204	7	$\chi_{\text{CC}\beta\text{CH}}(47.8)$ ; $\chi_{\text{CaC}\beta\text{CH}}(17.0)$	172 20 $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}(16.2)$ ; $\chi_{\text{CyCaC}\beta\text{F}}(16.2)$ ; $\chi_{\text{OPbOC}\alpha}(13.5)$
91	226	4	$\nu_{\text{HF}}(3.9)$ ; $\delta_{\text{CHF}}(3.7)$ ; $\chi_{\text{CC}\beta\text{CH}}(27.7)$ ; $\chi_{\text{CaC}\beta\text{CH}}(14.9)$ ; $\chi_{\text{C}\beta\text{CHF}}(7.0)$				
94	229	3	$\chi_{\text{CC}\beta\text{CH}}(28.3)$ ; $\chi_{\text{CaC}\beta\text{CH}}(14.3)$				
96	234	6	$\chi_{\text{CC}\beta\text{CH}}(30.6)$ ; $\chi_{\text{CaC}\beta\text{CH}}(16.2)$	231	3	$\chi_{\text{CC}\beta\text{CH}}(57.6)$ ; $\chi_{\text{CaC}\beta\text{CH}}(28.0)$	
102	247	5	$\chi_{\text{CC}\beta\text{CH}}(5.3)$ ; $\chi_{\text{FC}\beta\text{FH}}(5.2)$				
106	251	6	$\nu_{\text{HF}}(2.9)^*$ ; $\chi_{\text{FC}\beta\text{FH}}(8.3)$ ; $\chi_{\text{CH}/\text{HCFC}\beta}(5.8)$ ; $\chi_{\text{CC}\beta\text{CH}}(5.0)$ ; $\chi_{\text{CaC}\beta\text{FH}}(3.9)$ ; $\chi_{\text{HCHF}/\text{CHF}}(3.9)$ ; $\chi_{\text{C}\beta\text{CHF}}(3.3)$			245 2 $\delta_{\text{CaC}\beta\text{F}}(14.6)$ ; $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}(14.1)$	
108	253	2	$\chi_{\text{CC}\beta\text{CH}}(11)$ ; $\chi_{\text{CaC}\beta\text{CH}}(3.6)$				
111	260	8	$\chi_{\text{CC}\beta\text{CH}}(5.0)$ ; $\chi_{\text{OC}\alpha\text{C}\beta\text{F}}(4.7)$				
115	266	10	$\chi_{\text{CC}\beta\text{CH}}(15.8)$ ; $\chi_{\text{CaC}\beta\text{CH}}(8.4)$				
118	269	2	$\chi_{\text{CC}\beta\text{CH}}(12.9)$ ; $\chi_{\text{CaC}\beta\text{CH}}(10.2)$ ; $\chi_{\text{HCHF}/\text{CHF}}(4.0)$	269	14	$\chi_{\text{CC}\beta\text{CH}}(60.3)$ ; $\chi_{\text{CaC}\beta\text{CH}}(37.5)$	247 3 $\nu_{\text{PbO}}(9.1)$ ; $\delta_{\text{CaC}\beta\text{F}}(16.0)$

119	270	6	$\chi_{\text{CC}\beta\text{CH}}$ (27.1); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (14.0)			
122	273	12	$\chi_{\text{CC}\beta\text{CH}}$ (6.7); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (5.4); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (4.0)			
123	274	16	$\nu_{\text{HF}}$ (2.9)*; $\chi_{\text{CC}\beta\text{CH}}$ (23.2); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (11.4)			
125	279	3	$\chi_{\text{CC}\beta\text{CH}}$ (26.4); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (13.2); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (3.1)			
126	279	10	$\chi_{\text{CC}\beta\text{CH}}$ (24.7); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (12.8)			
128	289	5	$\chi_{\text{CC}\beta\text{CH}}$ (34.3); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (15.8)			
130	289	2	$\chi_{\text{CC}\beta\text{CH}}$ (32.4); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (14.6)	292	40	$\chi_{\text{CC}\beta\text{CH}}$ (50.4); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (25.6)
132	297	2	$\nu_{\text{OH}}$ (3.8); $\chi_{\text{CC}\beta\text{CH}}$ (17.6); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (8.1); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (7.7)			
133	300	2	$\chi_{\text{CC}\beta\text{CH}}$ (17.8); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (12.1); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (8.4); $\chi_{\text{CH/HCF}\underline{\text{C}}\beta}$ (4.6);			
135	301	3	$\chi_{\text{CC}\beta\text{CH}}$ (25.8); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (14.0); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (4.8)			
137	309	18	$\chi_{\text{CC}\beta\text{CH}}$ (14.5); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (8.6)			
140	312	3	$\chi_{\text{CC}\beta\text{CH}}$ (5.3); $\chi_{\text{OC}\alpha\text{C}\gamma\text{Ca}}$ (4.7); $\chi_{\text{C}\beta\text{CaC}\gamma\text{Ca}}$ (3.2);			311 6 $\delta_{\text{CaC}\beta\text{F}}$ (16.6); $\chi_{\text{OC}\alpha\text{C}\gamma\text{Ca}}$ (17.2); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (14.0)
141	317	5	$\chi_{\text{CC}\beta\text{CH}}$ (19.8); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (7.0)	317	8	$\chi_{\text{CC}\beta\text{CH}}$ (31.2); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (15.2)
144	321	5	$\chi_{\text{CC}\beta\text{CH}}$ (13.6); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (6.5); $\chi_{\text{OC}\alpha\text{C}\gamma\text{Ca}}$ (4.4)			
145	325	6	$\chi_{\text{CC}\beta\text{CH}}$ (14.6); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (13.4); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (5.6); $\chi_{\text{CH/HCF}\underline{\text{C}}\beta}$ (5.2); $\chi_{\text{HCHO}}$ (3.9); $\chi_{\text{FC}\beta\text{FH}}$ (3.4)			
147	330	3	$\chi_{\text{CC}\beta\text{CH}}$ (22.6); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (10.1); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (5.1)			
150	332	3	$\chi_{\text{CH/HCF}\underline{\text{C}}\beta}$ (6.8); $\chi_{\text{CC}\beta\text{CH}}$ (5.7); $\chi_{\text{FC}\beta\text{FH}}$ (5.6);			331 6 $\nu_{\text{PbO}}$ (9.6); $\delta_{\text{CaC}\beta\text{F}}$ (27.2); $\delta_{\text{FC}\beta\text{F}}$ (11.0)
154	337	3	$\chi_{\text{CC}\beta\text{CH}}$ (28.1); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (13.0)			
159	357	2	$\nu_{\text{HF}}$ (3.3); $\chi_{\text{CC}\beta\text{CH}}$ (13.7); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (10.1); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (5.3); $\chi_{\text{CH/HCF}\underline{\text{C}}\beta}$ (3.1); $\chi_{\text{HCHO}}$ (3.0)			
160	357	3	$\nu_{\text{HF}}$ (2.9)*; $\chi_{\text{CC}\beta\text{CH}}$ (16.7); $\chi_{\text{HCHF/CHF}\underline{\text{H}}}$ (7.1); $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}$ (4.7);			

			$\chi_{\text{CH/HCF}\beta}$ (3.6); $\chi_{\text{HCHO}}$ (3.1);			
161	364	10	$\chi_{\text{CC}\beta\text{CH}}$ (5.0); $\chi_{\text{HCHF/CHF}\text{H}}$ (7.8); $\chi_{\text{CH/HCF}\beta}$ (3.6); $\chi_{\text{FC}\beta\text{FH}}$ (3.4)			
164	366	8	$\nu_{\text{PbO}}$ (3.1)			359 3 $\nu_{\text{PbO}}$ (11.2); $\delta_{\text{CaC}\beta\text{F}}$ (16.0); $\delta_{\text{OCaC}\gamma}$ (10.2); $\chi_{\text{OPbOCa}}$ (10.3);
166	372	11	$\chi_{\text{FC}\beta\text{FH}}$ (8.3); $\chi_{\text{CH/HCF}\beta}$ (5.4); $\chi_{\text{CaC}\beta\text{FH}}$ (3.9)			
173	396	3	$\delta_{\text{CC}\beta\text{C}}$ (3.6); $\chi_{\text{CaC}\beta\text{CH}}$ (5.1); $\chi_{\text{HCHF/CHF}\text{H}}$ (5.0); $\chi_{\text{CC}\beta\text{CH}}$ (4.1); $\chi_{\text{C}\gamma\text{CaC}\beta\text{C}}$ (3.1)	394	3	$\chi_{\text{CC}\beta\text{CH}}$ (24.8)
177	430	3	$\chi_{\text{HCHF/CHF}\text{H}}$ (9.4); $\chi_{\text{CC}\beta\text{CH}}$ (3.9); $\chi_{\text{CH/HCF}\beta}$ (3.5)			
180	432	9	$\chi_{\text{HCHF/CHF}\text{H}}$ (6.2); $\chi_{\text{CC}\beta\text{CH}}$ (5.9)	433	8	$\chi_{\text{CC}\beta\text{CH}}$ (25.6); $\chi_{\text{CaC}\beta\text{CH}}$ (16.0); $\chi_{\text{OCaC}\beta\text{C}}$ (10.4)
186	451	18	$\nu_{\text{CuO}}$ (3.5); $\chi_{\text{HCHF/CHF}\text{H}}$ (8.4); $\chi_{\text{CH/HCF}\beta}$ (3.6)	452	4	$\nu_{\text{CuO}}$ (6.8)*; $\chi_{\text{CC}\beta\text{CH}}$ (40.4)
188	453	4	$\nu_{\text{PbO}}$ (3.0); $\chi_{\text{HCHF/CHF}\text{H}}$ (4.6); $\chi_{\text{CH/HCF}\beta}$ (3.2); $\chi_{\text{FC}\beta\text{FH}}$ (3.0)			446 3 $\nu_{\text{PbO}}$ (10.9); $\delta_{\text{FC}\beta\text{F}}$ (23.4); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (10.6); $\chi_{\text{OCaC}\beta\text{F}}$ (10.4)
						467 12 $\nu_{\text{PbO}}$ (15.5); $\delta_{\text{FC}\beta\text{F}}$ (18.6)
						476 4 $\nu_{\text{PbO}}$ (15.0); $\delta_{\text{FC}\beta\text{F}}$ (20.8)
194	500	33	$\delta_{\text{OCaC}\gamma}$ (2.9)*; $\chi_{\text{CC}\beta\text{CH}}$ (9.4)	500	20	$\chi_{\text{CC}\beta\text{CH}}$ (35.2); $\chi_{\text{CaC}\beta\text{CH}}$ (13.6)
200	508	10	$\chi_{\text{CC}\beta\text{CH}}$ (12.5); $\chi_{\text{HCHF/CHF}\text{H}}$ (3.8)			
202	512	58	$\nu_{\text{CuO}}$ (4.0); $\chi_{\text{CC}\beta\text{CH}}$ (8.7); $\chi_{\text{HCHF/CHF}\text{H}}$ (6.9); $\chi_{\text{CH/HCF}\beta}$ (4.3)	515	54	$\nu_{\text{CuO}}$ (6.0)*; $\chi_{\text{CC}\beta\text{CH}}$ (48)
204	521	13	$\nu_{\text{HF}}$ (3.4); $\delta_{\text{FC}\beta\text{F}}$ (8.8); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (8.4); $\chi_{\text{OCaC}\beta\text{F}}$ (5.7); $\chi_{\text{OCaC}\gamma\text{Ca}}$ (5.3); $\chi_{\text{FC}\beta\text{FH}}$ (4.5); $\chi_{\text{PbOCaC}\gamma}$ (4.0)			516 16 $\delta_{\text{FC}\beta\text{F}}$ (18.2); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (19.8); $\chi_{\text{OCaC}\beta\text{F}}$ (13.8)
205	521	32	$\nu_{\text{HF}}$ (6.1); $\delta_{\text{C}\beta\text{FH}}$ (4.0); $\delta_{\text{FC}\beta\text{F}}$ (10.0); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (8.4); $\chi_{\text{OCaC}\gamma\text{Ca}}$ (6.6); $\chi_{\text{OCaC}\beta\text{F}}$ (6.2); $\chi_{\text{FC}\beta\text{FH}}$ (5.4); $\chi_{\text{C}\beta\text{CaC}\gamma\text{Ca}}$ (3.6)			
206	521	4	$\nu_{\text{HF}}$ (5.3); $\delta_{\text{FC}\beta\text{F}}$ (9.3); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (7.5); $\chi_{\text{OCaC}\gamma\text{Ca}}$ (6.5); $\chi_{\text{OCaC}\beta\text{F}}$ (5.8); $\chi_{\text{FC}\beta\text{FH}}$ (4.3); $\chi_{\text{PbOCaC}\gamma}$ (3.3)			
208	569	10	$\nu_{\text{HF}}$ (3.2); $\nu_{\text{C}\beta\text{F}}$ (4.1); $\delta_{\text{FC}\beta\text{F}}$ (10.8); $\chi_{\text{OCaC}\beta\text{F}}$ (8.4); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (8.1);			567 6 $\nu_{\text{C}\beta\text{F}}$ (15.0); $\delta_{\text{FC}\beta\text{F}}$ (16.8); $\chi_{\text{C}\gamma\text{CaC}\beta\text{F}}$ (15.4);





270	893	166	$\nu_{\text{C}\alpha\text{C}\beta}(4.9)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(8.0)$ ; $\chi_{\text{HCHO}}(3.9)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(3.5)$			
271	947	6	$\nu_{\text{C}\beta\text{C}}(6.2)$ ; $\delta_{\text{C}\beta\text{CH}}(11.7)$ ; $\chi_{\text{CC}\beta\text{CH}}(10.2)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(9.9)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(5.9)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(3.9)$ ; $\chi_{\text{FC}\beta\text{FH}}(3.2)$	944	4	$\nu_{\text{C}\beta\text{C}}(10.4)$ ; $\delta_{\text{C}\beta\text{CH}}(23.2)$ ; $\chi_{\text{CC}\beta\text{CH}}(23.2)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(11.6)$
274	949	3	$\delta_{\text{HCH}}(14.6)$ ; $\nu_{\text{C}\beta\text{C}}(9.6)$ ; $\delta_{\text{C}\beta\text{CH}}(8.3)$ ; $\chi_{\text{CC}\beta\text{CH}}(17.3)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(10.6)$			
275	951	5	$\nu_{\text{C}\beta\text{C}}(7.5)$ ; $\delta_{\text{HCH}}(3.4)$ ; $\delta_{\text{C}\beta\text{CH}}(15.9)$ ; $\chi_{\text{CC}\beta\text{CH}}(18.8)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(9.9)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(4.9)$	951	6	$\nu_{\text{C}\beta\text{C}}(11.6)$ ; $\delta_{\text{C}\beta\text{CH}}(27.6)$ ; $\chi_{\text{CC}\beta\text{CH}}(25.6)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(10.4)$
276	951	4	$\nu_{\text{C}\beta\text{C}}(7.5)$ ; $\delta_{\text{C}\beta\text{CH}}(15.9)$ ; $\delta_{\text{HCH}}(3.4)$ ; $\chi_{\text{CC}\beta\text{CH}}(18.6)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(9.9)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(4.9)$			
277	952	5	$\nu_{\text{C}\beta\text{C}}(7.3)$ ; $\delta_{\text{C}\beta\text{CH}}(14.3)$ ; $\chi_{\text{CC}\beta\text{CH}}(12.1)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(7.6)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(7.3)$ ; $\chi_{\text{HCHO}}(6.0)$			
279	953	2	$\nu_{\text{C}\beta\text{C}}(4.8)$ ; $\delta_{\text{C}\beta\text{CH}}(7.6)$ ; $\delta_{\text{HCH}}(5.0)$ ; $\chi_{\text{CC}\beta\text{CH}}(12.9)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(9.5)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(6.7)$ ; $\chi_{\text{C}\alpha\text{OH}\text{C}}(4.0)$ ; $\chi_{\text{PbOH}\text{C}}(3.2)$			
280	953	3	$\nu_{\text{C}\beta\text{C}}(3.7)$ ; $\delta_{\text{C}\beta\text{CH}}(8.0)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(20.7)$ ; $\chi_{\text{CC}\beta\text{CH}}(9.8)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(5.3)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(5.2)$ ; $\chi_{\text{C}\beta\text{CHF}}(4.5)$ ; $\chi_{\text{C}\alpha\text{OH}\text{C}}(3.1)$			
281	956	2	$\nu_{\text{C}\beta\text{C}}(6.4)$ ; $\delta_{\text{C}\beta\text{CH}}(14.9)$ ; $\chi_{\text{CC}\beta\text{CH}}(12.9)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(7.7)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(6.6)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(6.2)$ ; $\chi_{\text{FC}\beta\text{FH}}(3.6)$			
282	956	3	$\nu_{\text{C}\beta\text{C}}(6.4)$ ; $\delta_{\text{C}\beta\text{CH}}(15.0)$ ; $\chi_{\text{CC}\beta\text{CH}}(13.0)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(7.9)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(6.5)$ ; $\chi_{\text{FC}\beta\text{FH}}(3.6)$			
288	962	3	$\delta_{\text{OC}\alpha\text{C}\gamma}(8.1)$ ; $\delta_{\text{C}\alpha\text{C}\gamma\text{C}\alpha}(5.4)$ ; $\delta_{\text{C}\alpha\text{C}\gamma\text{H}\alpha}(5.4)$ ; $\delta_{\text{C}\gamma\text{C}\alpha\text{C}\beta}(5.2)$	961	2	$\nu_{\text{C}\beta\text{F}}(10.6)$ ; $\delta_{\text{OC}\alpha\text{C}\gamma}(13.6)$
289	963	4	$\nu_{\text{C}\alpha\text{C}\gamma}(3.0)$ ; $\delta_{\text{OC}\alpha\text{C}\gamma}(8.2)$ ; $\delta_{\text{C}\alpha\text{C}\gamma\text{C}\alpha}(5.7)$ ; $\delta_{\text{C}\alpha\text{C}\gamma\text{H}\alpha}(5.7)$ ; $\delta_{\text{C}\gamma\text{C}\alpha\text{C}\beta}(5.3)$ ; $\delta_{\text{PbOC}\alpha}(3.1)$ ; $\chi_{\text{OCuOC}\alpha}(4.0)$			
296	981	11	$\delta_{\text{C}\beta\text{CH}}(9.6)$ ; $\chi_{\text{HC/CHF}\text{C}\beta}(3.1)$			
298	982	2	$\delta_{\text{C}\beta\text{CH}}(15.0)$ ; $\chi_{\text{CC}\beta\text{CH}}(13.8)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(6.6)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(3.7)$	983	10	$\delta_{\text{C}\beta\text{CH}}(13.7)$ ; $\chi_{\text{CC}\beta\text{CH}}(12.8)$
299	983	3	$\delta_{\text{C}\beta\text{CH}}(10.8)$ ; $\chi_{\text{CC}\beta\text{CH}}(10.3)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(5.0)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(3.4)$ ; $\chi_{\text{HCHO}}(3.0)$			
303	1050	4	$\delta_{\text{C}\beta\text{CH}}(11.8)$ ; $\delta_{\text{HCH}}(4.3)$ ; $\chi_{\text{HCHF/CHF}\text{H}}(13.2)$ ; $\chi_{\text{CC}\beta\text{CH}}(12.0)$ ; $\chi_{\text{C}\alpha\text{C}\beta\text{CH}}(7.2)$ ; $\chi_{\text{CH/HCF}\text{C}\beta}(5.7)$ ; $\chi_{\text{HCHO}}(3.1)$			

304	1050	4	$\delta\text{C}\beta\text{CH}(14.0)$ ; $\chi\text{CC}\beta\text{CH}(12.6)$ ; $\chi\text{HCHF/CHF}\text{H}(10.9)$ ; $\chi\text{C}\alpha\text{C}\beta\text{CH}(7.5)$ ; $\chi\text{CH/HCF}\beta(5.7)$ ; $\chi\text{HCHO}(3.2)$		
305	1056	6	$\delta\text{C}\beta\text{CH}(17.8)$ ; $\chi\text{CC}\beta\text{CH}(15.3)$ ; $\chi\text{C}\alpha\text{C}\beta\text{CH}(10.3)$ ; $\chi\text{HCHF/CHF}\text{H}(3.2)$	1054	4 $\delta\text{C}\beta\text{CH}(28.0)$ ; $\chi\text{CC}\beta\text{CH}(25.6)$ ; $\chi\text{C}\alpha\text{C}\beta\text{CH}(14.4)$
314	1065	3	$\delta\text{C}\beta\text{CH}(14.0)$ ; $\chi\text{HCHF/CHF}\text{H}(11.9)$ ; $\chi\text{CC}\beta\text{CH}(11.0)$ ; $\chi\text{C}\alpha\text{C}\beta\text{CH}(5.6)$ ; $\chi\text{CH/HCF}\beta(5.2)$ ; $\chi\text{HCHO}(3.6)$		

### S3 Optimised Geometries

*Cartesian coordinates in units of  $10^{-10}$  m.*

#### 1(T) – BS1

Pb	1.89274400	0.37323300	-0.74349400
Cu	5.16787000	-0.28058800	-0.96290400
O	2.38524400	2.64911000	0.01669000
O	0.72491200	0.63653700	1.35006000
O	3.54707500	0.10762000	0.89927100
O	1.51414600	-1.84797600	0.17909200
O	6.53196200	0.90011500	-0.31775000
O	4.25346800	1.12854600	-1.94471200
O	5.92802700	-1.75178100	0.02952400
O	3.89164600	-1.44063200	-1.86526300
C	2.40615900	3.08625500	1.18714400
C	1.77994000	2.55903200	2.33181200
H	1.91509600	3.07455000	3.27429500
C	1.01720200	1.39827100	2.32206900
C	3.28649500	4.33759000	1.38057900
C	0.51419300	0.89919400	3.68969200
C	3.61975100	-0.68189700	1.89120900
C	2.92854500	-1.86830300	2.11166600
H	3.13785400	-2.42748300	3.01411800
C	1.97097400	-2.37663300	1.21629800
C	4.60017400	-0.20489000	2.97741700
C	1.41516500	-3.78615100	1.50477700
C	6.60796700	2.15452700	-0.53430300
C	5.75381900	2.87876500	-1.38934300
H	5.96855400	3.92641700	-1.53389600
C	4.67190900	2.34347400	-2.08492100
C	7.77821500	2.84914400	0.18291900
C	7.70822800	2.48500100	1.68073700
H	7.75495400	1.40135000	1.81980900
H	6.77576700	2.84946900	2.13045700
H	8.55171700	2.94903900	2.21005500
C	9.08123300	2.28361900	-0.42428800
H	9.95098000	2.71671000	0.08863700
H	9.15794600	2.52893900	-1.49307700
H	9.11544100	1.19329000	-0.31371200
C	7.76152200	4.37865900	0.03703600
H	8.58912900	4.80546000	0.61911000
H	6.82494600	4.80624100	0.41684900
H	7.89572500	4.69638400	-1.00571800
C	3.97184300	3.15510100	-3.18705600
C	4.66322700	2.72846200	-4.50637200
H	4.55280300	1.64838800	-4.66938800
H	5.73403700	2.97110000	-4.48706700
H	4.20434400	3.25640100	-5.35378100
C	4.11966900	4.67401500	-2.99384900
H	3.52823900	5.19524100	-3.75822300

H	5.15974500	5.00581100	-3.10632800
H	3.75709900	4.98676500	-2.00762900
C	2.47570300	2.80923000	-3.27995700
H	2.32535700	1.73974400	-3.46599200
H	2.02859700	3.35568100	-4.12106300
H	1.94278700	3.10345900	-2.36851700
C	5.64435900	-2.98736100	-0.11178800
C	4.75406200	-3.50036500	-1.07442100
H	4.68105300	-4.57407400	-1.16548800
C	3.97582600	-2.72466100	-1.93533500
C	6.42613500	-3.93767500	0.81133700
C	7.85727500	-4.02973900	0.23387000
H	8.47480400	-4.68163800	0.86709000
H	8.32109500	-3.03614600	0.19741800
H	7.84728800	-4.44816800	-0.78212700
C	5.80276100	-5.34138000	0.89102100
H	5.88522800	-5.88749100	-0.05790400
H	4.74196600	-5.29386700	1.17123800
H	6.33099600	-5.93023200	1.65260800
C	6.48538500	-3.33365900	2.22694000
H	7.12025800	-3.96103400	2.86694000
H	5.48652200	-3.29183600	2.67912500
H	6.89486700	-2.31971400	2.20720500
C	3.12720400	-3.38235100	-3.03840200
C	3.68376000	-4.75310700	-3.46420000
H	3.59884000	-5.50259300	-2.66721100
H	4.73741400	-4.68466500	-3.76605200
H	3.10728000	-5.12464200	-4.32193600
C	1.69442000	-3.57099500	-2.49888000
H	1.04009700	-3.94025200	-3.29906700
H	1.28788500	-2.63021400	-2.12017800
H	1.67365900	-4.28847900	-1.66991100
C	3.10593600	-2.45244600	-4.26762100
H	2.46910500	-2.88949800	-5.04797000
H	4.11710000	-2.32504100	-4.67910400
H	2.71672700	-1.46327500	-4.01497900
F	3.01687300	4.99885500	2.52300900
F	4.58722700	3.97106500	1.41811200
F	3.13011300	5.19905800	0.36147400
F	-0.65371700	0.22520000	3.56592700
F	0.31410100	1.89279300	4.57328100
F	1.41080100	0.04498000	4.22215600
F	5.82009000	0.01235300	2.46540100
F	4.72599200	-1.08644000	3.99030300
F	4.16263400	0.95900800	3.50298400
F	2.13087300	-4.70690600	0.81611700
F	0.13441100	-3.88722800	1.11362300
F	1.47865700	-4.11325900	2.80932600
Pb	-1.89379200	-0.37190800	0.74204700
Cu	-5.16828400	0.28011500	0.96586700
O	-2.38525400	-2.64763400	-0.01793400

O	-0.72652300	-0.63425900	-1.35188300
O	-3.54998700	-0.10874000	-0.89938900
O	-1.51915800	1.84932500	-0.18131500
O	-6.53138000	-0.90211600	0.32132600
O	-4.25121100	-1.12851800	1.94647600
O	-5.93056300	1.75006800	-0.02704700
O	-3.89332700	1.44172900	1.86754600
C	-2.40591900	-3.08523100	-1.18819300
C	-1.78009700	-2.55788700	-2.33301400
H	-1.91491800	-3.07374000	-3.27538600
C	-1.01847700	-1.39638200	-2.32366000
C	-3.28558800	-4.33709500	-1.38113000
C	-0.51683900	-0.89724200	-3.69174000
C	-3.62363700	0.67951900	-1.89218400
C	-2.93277400	1.86583100	-2.11456900
H	-3.14235700	2.42357300	-3.01782900
C	-1.97545200	2.37578900	-1.21991800
C	-4.60507600	0.20110100	-2.97689300
C	-1.41874400	3.78443300	-1.51061400
C	-6.60572900	-2.15666700	0.53750200
C	-5.74995300	-2.88025800	1.39150300
H	-5.96339100	-3.92820300	1.53567600
C	-4.66812700	-2.34403600	2.08647200
C	-7.77595200	-2.85242700	-0.17870300
C	-7.70852300	-2.48724700	-1.67637700
H	-7.75704300	-1.40358800	-1.81467400
H	-6.77613700	-2.85001600	-2.12761900
H	-8.55204900	-2.95220500	-2.20482100
C	-9.07890600	-2.28901400	0.43061800
H	-9.94876700	-2.72298000	-0.08137600
H	-9.15384000	-2.53505100	1.49936800
H	-9.11474800	-1.19866600	0.32071700
C	-7.75705100	-4.38201200	-0.03380000
H	-8.58478500	-4.80953900	-0.61516100
H	-6.82036700	-4.80811600	-0.41499000
H	-7.88961700	-4.70058800	1.00890400
C	-3.96606500	-3.15530900	3.18764600
C	-4.65231700	-2.72529900	4.50851300
H	-4.53921400	-1.64521100	4.66948600
H	-5.72367800	-2.96583000	4.49301900
H	-4.19179700	-3.25290200	5.35524200
C	-4.11742400	-4.67422200	2.99731000
H	-3.52504300	-5.19540900	3.76096700
H	-5.15787700	-5.00371800	3.11302100
H	-3.75799600	-4.98930500	2.01066300
C	-2.46882000	-2.81250500	3.27514800
H	-2.31533500	-1.74333900	3.46049300
H	-2.01997100	-3.35963000	4.11488700
H	-1.93991500	-3.10811300	2.36186100
C	-5.64676900	2.98584300	0.11229500
C	-4.75601100	3.50025100	1.07373400

H	-4.68301800	4.57409100	1.16316000
C	-3.97750000	2.72587200	1.93554800
C	-6.42905100	3.93513100	-0.81151600
C	-7.85917800	4.02974200	-0.23195100
H	-8.47703300	4.68115300	-0.86535700
H	-8.32399700	3.03670700	-0.19299200
H	-7.84715100	4.44996900	0.78328000
C	-5.80434900	5.33806300	-0.89474600
H	-5.88537700	5.88629500	0.05307200
H	-4.74383900	5.28895900	-1.17580600
H	-6.33270700	5.92582400	-1.65709100
C	-6.49123600	3.32867100	-2.22593200
H	-7.12648900	3.95561500	-2.86597700
H	-5.49316700	3.28502600	-2.67969000
H	-6.90174300	2.31521000	-2.20376900
C	-3.12848400	3.38517100	3.03733800
C	-3.68163700	4.75881300	3.45811800
H	-3.59408300	5.50536700	2.65866200
H	-4.73567700	4.69425200	3.75949800
H	-3.10473900	5.13162100	4.31501900
C	-1.69468800	3.56822700	2.49860800
H	-1.04004000	3.93812100	3.29825200
H	-1.29071700	2.62496800	2.12350400
H	-1.67107900	4.28289300	1.66731400
C	-3.11083300	2.45903400	4.26946600
H	-2.47364700	2.89680200	5.04914300
H	-4.12272800	2.33553000	4.68036000
H	-2.72382500	1.46819600	4.01996000
F	-3.01532700	-4.99886500	-2.52312200
F	-4.58645900	-3.97116100	-1.41921300
F	-3.12912200	-5.19792300	-0.36149200
F	0.64662000	-0.21580000	-3.56824900
F	-0.30985000	-1.89177600	-4.57276900
F	-1.41815200	-0.04987400	-4.22736000
F	-5.82519400	-0.01272100	-2.46380400
F	-4.72984100	1.08024600	-3.99199900
F	-4.16976900	-0.96486500	-3.49952400
F	-2.12855000	4.70596000	-0.81704200
F	-0.13543800	3.88241200	-1.12657500
F	-1.48886100	4.11303700	-2.81440600

**1(T) – BS2**

Pb	1.96335100	0.25899600	-0.66136000
Cu	5.23268800	-0.40852500	-0.89727100
O	2.42119500	2.55571800	0.09126900
O	0.71878100	0.58972400	1.40753500
O	3.58884000	-0.01713800	0.99166000
O	1.47147200	-1.94577000	0.31488000
O	6.58865100	0.78508900	-0.26629000
O	4.29255800	0.99881800	-1.86212600
O	6.06705700	-1.86308800	0.05308000

O	3.91509200	-1.59750900	-1.70236000
C	2.38282900	3.03649000	1.24284400
C	1.76898800	2.50878900	2.39620100
H	1.88805300	3.03947400	3.33290300
C	1.01155000	1.34422800	2.38519700
C	3.15242000	4.37224500	1.39678500
C	0.46653200	0.84239000	3.74196100
C	3.66294600	-0.82215500	1.97328500
C	2.97537200	-2.00974300	2.18269100
H	3.20477900	-2.58771000	3.07071000
C	1.96816500	-2.49103300	1.32030000
C	4.64931700	-0.35286100	3.06436800
C	1.40526400	-3.89514200	1.66287700
C	6.68629700	2.02972100	-0.52179400
C	5.82620500	2.74424000	-1.38114000
H	6.05470900	3.78417000	-1.56006100
C	4.72080300	2.20764200	-2.03915000
C	7.87800500	2.71945400	0.16462900
C	7.73888700	2.49357000	1.68608100
H	7.71480400	1.42459300	1.92064100
H	6.81717300	2.95105500	2.07159900
H	8.59334100	2.95222400	2.20472600
C	9.16436500	2.03043200	-0.34284200
H	10.04072500	2.46091200	0.16323000
H	9.29076000	2.17599700	-1.42617700
H	9.13345700	0.95340100	-0.13839300
C	7.96214700	4.22774200	-0.11543800
H	8.81997900	4.64675200	0.42956700
H	7.06097000	4.75671800	0.22393300
H	8.11432200	4.44222800	-1.18302600
C	4.00309500	3.00637600	-3.14060900
C	4.65512800	2.54742200	-4.46980100
H	4.53071800	1.46532900	-4.61204300
H	5.72908400	2.78037600	-4.48616700
H	4.17613600	3.06522100	-5.31379100
C	4.17042600	4.52801400	-2.98417800
H	3.57356500	5.03643900	-3.75449400
H	5.21213900	4.84961300	-3.11690300
H	3.81910800	4.86964400	-2.00234500
C	2.50070000	2.67850100	-3.18792300
H	2.33046100	1.61035100	-3.36053500
H	2.03543000	3.22262600	-4.02170900
H	1.99835200	2.98978300	-2.26422100
C	5.86694100	-3.10744700	-0.13514600
C	4.94219700	-3.63720800	-1.05889300
H	4.92832100	-4.70835800	-1.19363000
C	4.05149900	-2.87576300	-1.81902500
C	6.75699800	-4.02488100	0.72045500
C	8.22633900	-3.70578400	0.36593600
H	8.89933100	-4.30600600	0.99530900
H	8.44237900	-2.64345100	0.53077500

H	8.43998500	-3.94518500	-0.68646400
C	6.48967600	-5.52157000	0.50109300
H	6.70301900	-5.83210300	-0.53168900
H	5.45118100	-5.79057600	0.74020500
H	7.14557800	-6.10527000	1.16249700
C	6.49879000	-3.67673400	2.20245300
H	7.14796400	-4.28907100	2.84466600
H	5.45497700	-3.88216400	2.47911400
H	6.70962500	-2.62010400	2.39751000
C	3.16855600	-3.52434900	-2.89939100
C	3.49621600	-5.00628200	-3.14393400
H	3.29190700	-5.62525800	-2.25912500
H	4.54519000	-5.15061700	-3.43831400
H	2.86390500	-5.38285500	-3.96041000
C	1.68992000	-3.41019400	-2.48327400
H	1.04778900	-3.77313400	-3.29781000
H	1.42129400	-2.37378600	-2.26933400
H	1.47426000	-4.00132200	-1.58474200
C	3.39950600	-2.73582400	-4.20886100
H	2.76242700	-3.14674500	-5.00491200
H	4.44751300	-2.81406100	-4.53426000
H	3.15786700	-1.67569100	-4.07880400
F	2.83911400	5.03985000	2.53039000
F	4.48514900	4.13624400	1.42237300
F	2.90043600	5.19315700	0.35918900
F	-0.81729500	0.42259900	3.62561800
F	0.49586200	1.77394800	4.71588700
F	1.19128300	-0.21693000	4.16684800
F	5.87686600	-0.14867400	2.56160100
F	4.76467300	-1.23010400	4.08787800
F	4.22020600	0.82075400	3.58792400
F	2.33484100	-4.84830100	1.39492100
F	0.30758900	-4.18137100	0.94915200
F	1.08820500	-3.99981000	2.97515100
Pb	-1.93500700	-0.18259600	0.60215300
Cu	-5.22287600	0.36858400	0.90970900
O	-2.37169600	-2.47574700	-0.19107300
O	-0.70557300	-0.46563200	-1.47981900
O	-3.59470400	0.08031800	-1.02475700
O	-1.51306500	2.03252100	-0.34566000
O	-6.55166500	-0.86115300	0.29219200
O	-4.21840800	-1.01744100	1.83873200
O	-6.12923900	1.80209800	-0.00472000
O	-3.93152200	1.59461900	1.70118400
C	-2.35247200	-2.92515100	-1.35487900
C	-1.76222800	-2.36227700	-2.50466500
H	-1.89307900	-2.86889500	-3.45305600
C	-1.00657800	-1.19767200	-2.47277800
C	-3.11932800	-4.25928000	-1.53591200
C	-0.45882200	-0.66760400	-3.81675700
C	-3.70634600	0.90203200	-1.98694600

C	-3.04279500	2.10627500	-2.19088300
H	-3.29812500	2.69249100	-3.06552000
C	-2.02620300	2.58517100	-1.34057800
C	-4.69770900	0.43006500	-3.07287200
C	-1.47394400	4.00125600	-1.64350400
C	-6.59992000	-2.11242800	0.52759800
C	-5.69556500	-2.81056000	1.35474700
H	-5.88243500	-3.86124900	1.51848100
C	-4.59950300	-2.24386800	2.00323900
C	-7.78973100	-2.82946600	-0.13372500
C	-7.74985400	-2.52224900	-1.64629200
H	-7.78763500	-1.44294500	-1.82597500
H	-6.83260300	-2.91499000	-2.10616300
H	-8.61156800	-2.99519700	-2.13937200
C	-9.07759700	-2.23326300	0.47826400
H	-9.95934400	-2.68509100	0.00088600
H	-9.13356900	-2.43526400	1.55841400
H	-9.11240800	-1.14764600	0.32529000
C	-7.78331100	-4.35196700	0.07280800
H	-8.63857100	-4.79038900	-0.46086500
H	-6.86894100	-4.81309300	-0.32495300
H	-7.88253600	-4.62649300	1.13278100
C	-3.83165800	-3.03014100	3.07961700
C	-4.43353600	-2.56929600	4.43142900
H	-4.31300700	-1.48552900	4.56244800
H	-5.50398900	-2.81149300	4.49211400
H	-3.91678900	-3.07856100	5.25811800
C	-3.99100500	-4.55399100	2.93998800
H	-3.36437000	-5.05143100	3.69357200
H	-5.02522400	-4.88241800	3.11000500
H	-3.66980200	-4.90071500	1.94949900
C	-2.33105300	-2.68937000	3.06379600
H	-2.16294300	-1.62068900	3.23617800
H	-1.82428600	-3.23352200	3.87263600
H	-1.86815500	-2.98979500	2.11634900
C	-5.97664000	3.05032600	0.20323700
C	-5.05428500	3.60142900	1.11614500
H	-5.07988400	4.66992600	1.26891500
C	-4.11504100	2.86450200	1.84179900
C	-6.92415100	3.94425400	-0.61458100
C	-8.36955200	3.56868000	-0.21887300
H	-9.08286500	4.15060000	-0.82044400
H	-8.55238300	2.50096600	-0.38933000
H	-8.55884700	3.78927400	0.84224200
C	-6.70397400	5.44716000	-0.38581600
H	-6.90001500	5.73947300	0.65564300
H	-5.68230000	5.75545800	-0.64903600
H	-7.39762600	6.01405700	-1.02287600
C	-6.69974000	3.62034700	-2.10729100
H	-7.38756000	4.21720100	-2.72329500
H	-5.67194200	3.86222900	-2.41336300

H	-6.88113700	2.55924800	-2.30782600
C	-3.23181200	3.53148800	2.91076900
C	-3.61359900	4.99454300	3.18860400
H	-3.45652500	5.63547100	2.30987700
H	-4.65992300	5.09063200	3.51085800
H	-2.97711500	5.38341800	3.99603600
C	-1.76068300	3.48700400	2.45525900
H	-1.11324200	3.85919900	3.26123900
H	-1.45505400	2.46776100	2.21034300
H	-1.59567500	4.10636300	1.56525800
C	-3.39748400	2.71365300	4.21208300
H	-2.75575700	3.13605000	4.99827900
H	-4.43882700	2.74633900	4.56551400
H	-3.11925500	1.66590700	4.05822900
F	-2.76465400	-4.92623600	-2.65806100
F	-4.44973000	-4.01848200	-1.61330900
F	-2.91055900	-5.08185100	-0.49125600
F	0.85399500	-0.34222100	-3.70849700
F	-0.56917000	-1.54561700	-4.83320500
F	-1.11618100	0.45820600	-4.17354800
F	-5.88152900	0.08774300	-2.54451100
F	-4.92410100	1.36218100	-4.02674000
F	-4.19336700	-0.66453600	-3.69494800
F	-2.22583100	4.93057800	-0.99795500
F	-0.20724900	4.13537300	-1.21997400
F	-1.50473100	4.30353200	-2.96117300

1(S) – BS1

Pb	1.86901600	0.37816100	-0.67281500
Cu	5.15565900	-0.21781500	-0.88110500
O	2.40608000	2.63747600	0.17434000
O	0.67863800	0.62112400	1.41141200
O	3.50269400	0.09369700	0.98004400
O	1.42857700	-1.82523600	0.22970500
O	6.54423300	0.97665700	-0.28767000
O	4.22557100	1.18422300	-1.88767900
O	5.94403700	-1.66403200	0.17172300
O	3.86029500	-1.43513200	-1.71190300
C	2.50011000	2.96991900	1.37348100
C	1.83807800	2.42398200	2.49243100
H	2.01202400	2.87490100	3.46166400
C	0.99197300	1.32545600	2.41976600
C	3.53538100	4.07615000	1.66444600
C	0.40742900	0.80992500	3.74762800
C	3.61701900	-0.75664600	1.91185400
C	2.92474200	-1.95031900	2.09578000
H	3.17861200	-2.56614200	2.94911800
C	1.92736700	-2.40676300	1.21952800
C	4.62898400	-0.35640300	2.99888600
C	1.38912500	-3.83268700	1.45477100
C	6.58768900	2.23167200	-0.48670300

C	5.69690000	2.95482600	-1.30521700
H	5.88447900	4.01019000	-1.42927700
C	4.62106000	2.40611200	-2.00188700
C	7.78444700	2.93993700	0.18168900
C	7.94383700	2.40535700	1.61842100
H	8.04429300	1.31556600	1.62165500
H	7.07633700	2.67117300	2.23413100
H	8.83997100	2.84764500	2.07470800
C	9.03167300	2.56306700	-0.64988700
H	9.92682000	3.02185800	-0.20759000
H	8.94009300	2.92001900	-1.68523100
H	9.16922800	1.47481300	-0.66697900
C	7.63132800	4.46898100	0.22461500
H	8.46208700	4.89816200	0.80060200
H	6.69228400	4.76138400	0.71037500
H	7.66263100	4.91842600	-0.77674500
C	3.89547700	3.22923200	-3.08536400
C	4.57800800	2.83957500	-4.41935600
H	4.48600300	1.76078300	-4.60072800
H	5.64419300	3.10225400	-4.40863200
H	4.09863500	3.37371700	-5.25145400
C	4.01914400	4.74594800	-2.86219500
H	3.41085900	5.27127300	-3.61041700
H	5.05187800	5.09894100	-2.97711100
H	3.66000300	5.03105800	-1.86632500
C	2.40399800	2.86118200	-3.16264800
H	2.26553400	1.79543200	-3.37590500
H	1.93242200	3.42486800	-3.97868700
H	1.88445000	3.12204200	-2.23361700
C	5.74449300	-2.90466800	-0.00802000
C	4.85626000	-3.45185200	-0.96052400
H	4.85169800	-4.52757900	-1.06686400
C	4.01378600	-2.71313100	-1.78952800
C	6.55607900	-3.86088000	0.89064600
C	7.29305200	-4.89879900	0.01721100
H	7.92770500	-5.52573100	0.65830400
H	7.93862000	-4.40586700	-0.72233100
H	6.60337700	-5.56191500	-0.51864500
C	5.57544600	-4.57732100	1.84567300
H	4.76752200	-5.08407400	1.30391100
H	5.12408100	-3.85841300	2.53964600
H	6.11936700	-5.32599100	2.43810000
C	7.58734600	-3.07345700	1.71361700
H	8.15612700	-3.77047000	2.34413600
H	7.10376600	-2.33515800	2.36075200
H	8.29110400	-2.53913600	1.06323000
C	3.19564400	-3.39742500	-2.90527500
C	3.67177100	-4.82909300	-3.20064800
H	3.50035200	-5.50271400	-2.35093900
H	4.73828100	-4.85722000	-3.46062600
H	3.10431500	-5.22768000	-4.05224900

C	1.71393600	-3.44529100	-2.48337200
H	1.09710600	-3.77939900	-3.32808100
H	1.36491600	-2.46216000	-2.16320000
H	1.56115900	-4.13525200	-1.64570300
C	3.34562700	-2.54488500	-4.18333000
H	2.75745800	-2.99334000	-4.99523500
H	4.39613300	-2.50067800	-4.50411200
H	2.99381100	-1.52268800	-4.01986200
F	3.23368600	4.79502300	2.76420200
F	4.74332600	3.50079700	1.87279600
F	3.65875200	4.92856700	0.63654200
F	-0.84333400	0.31672000	3.57027800
F	0.33170600	1.75906400	4.69627800
F	1.16517500	-0.19716300	4.22246600
F	5.65698900	0.33018500	2.49544400
F	5.12404200	-1.43040000	3.65740000
F	4.01108200	0.42720100	3.91249800
F	2.13367600	-4.72105800	0.75305600
F	0.11892500	-3.94747000	1.03621100
F	1.43600400	-4.19584500	2.75077500
Pb	-1.86932100	-0.37735400	0.67124500
Cu	-5.15594500	0.21734900	0.88304900
O	-2.40559500	-2.63676200	-0.17461700
O	-0.67995100	-0.61980600	-1.41368800
O	-3.50480800	-0.09476100	-0.98007300
O	-1.43194500	1.82641200	-0.23170600
O	-6.54406900	-0.97785500	0.29038900
O	-4.22426500	-1.18430100	1.88874900
O	-5.94570900	1.66265100	-0.17003700
O	-3.86161700	1.43556200	1.71362200
C	-2.49920300	-2.97060200	-1.37339000
C	-1.83793700	-2.42486700	-2.49285400
H	-2.01142900	-2.87682500	-3.46167600
C	-0.99291800	-1.32538700	-2.42127300
C	-3.53280000	-4.07875800	-1.66283800
C	-0.40897900	-0.81054100	-3.74964600
C	-3.61971100	0.75449100	-1.91276400
C	-2.92797300	1.94825300	-2.09821700
H	-3.18205300	2.56278700	-2.95240200
C	-1.93065000	2.40611100	-1.22265800
C	-4.63168900	0.35271400	-2.99919300
C	-1.39224600	3.83163000	-1.45993300
C	-6.58678000	-2.23291300	0.48938900
C	-5.69511700	-2.95563900	1.30732500
H	-5.88206700	-4.01108700	1.43141600
C	-4.61915700	-2.40635700	2.00336000
C	-7.78368000	-2.94167700	-0.17820900
C	-7.94319600	-2.40831600	-1.61538400
H	-8.04375100	-1.31853900	-1.61950500
H	-7.07569000	-2.67459200	-2.23091000
H	-8.83931700	-2.85108200	-2.07122300

C	-9.03075200	-2.56392600	0.65320100
H	-9.92599900	-3.02304400	0.21145500
H	-8.93905700	-2.91993900	1.68886100
H	-9.16818700	-1.47564400	0.66932300
C	-7.63081400	-4.47077200	-0.21989600
H	-8.46173900	-4.90026100	-0.79541900
H	-6.69190500	-4.76370900	-0.70558600
H	-7.66206400	-4.91944300	0.78181000
C	-3.89240500	-3.22895200	3.08645500
C	-4.57096300	-2.83577800	4.42142800
H	-4.47653000	-1.75686100	4.60072000
H	-5.63766300	-3.09652100	4.41374800
H	-4.09057500	-3.36941900	5.25326100
C	-4.01941300	-4.74580500	2.86627600
H	-3.41058300	-5.27094900	3.61417400
H	-5.05260000	-5.09656400	2.98396400
H	-3.66284500	-5.03345200	1.87018100
C	-2.40004300	-2.86351900	3.15944800
H	-2.25911700	-1.79785300	3.37144900
H	-1.92739800	-3.42726400	3.97483500
H	-1.88340700	-3.12604600	2.22930600
C	-5.74568500	2.90347900	0.00802700
C	-4.85689700	3.45160200	0.95942700
H	-4.85198400	4.52746000	1.06438600
C	-4.01471100	2.71370500	1.78945500
C	-6.55745300	3.85888500	-0.89126000
C	-7.29496300	4.89676600	-0.01830600
H	-7.92910500	5.52390300	-0.65972600
H	-7.94114600	4.40385800	0.72072300
H	-6.60553800	5.55965400	0.51815400
C	-5.57700400	4.57556500	-1.84639200
H	-4.77008100	5.08381200	-1.30453600
H	-5.12427300	3.85665700	-2.53943500
H	-6.12152200	5.32307700	-2.43972400
C	-7.58812400	3.07068300	-1.71419300
H	-8.15759700	3.76726800	-2.34455300
H	-7.10394700	2.33289300	-2.36146800
H	-8.29130100	2.53566900	-1.06376700
C	-3.19633100	3.39933100	2.90419200
C	-3.67208300	4.83149000	3.19770400
H	-3.50071000	5.50391700	2.34704500
H	-4.73852600	4.86022700	3.45790500
H	-3.10432200	5.23110600	4.04861500
C	-1.71470500	3.44604000	2.48191400
H	-1.09753100	3.78153100	3.32582200
H	-1.36647200	2.46197300	2.16384800
H	-1.56183500	4.13415300	1.64275200
C	-3.34603300	2.54851900	4.18343400
H	-2.75906300	2.99910500	4.99503200
H	-4.39666100	2.50316400	4.50360800
H	-2.99240000	1.52664800	4.02176300

F	-3.23089900	-4.79767500	-2.76249500
F	-4.74201700	-3.50572300	-1.87030300
F	-3.65354600	-4.93080700	-0.63431300
F	0.84228000	-0.31827600	-3.57344800
F	-0.33474100	-1.75981700	-4.69829100
F	-1.16642000	0.19705500	-4.22397100
F	-5.65965400	-0.33325800	-2.49479600
F	-5.12686400	1.42581900	-3.65908000
F	-4.01373100	-0.43202400	-3.91176200
F	-2.13324600	4.72028900	-0.75484800
F	-0.12023000	3.94521400	-1.04652600
F	-1.44410200	4.19540800	-2.75556300

**1(S) – BS2**

Pb	1.96341700	0.24856600	-0.65452100
Cu	5.22371300	-0.41483900	-0.90818000
O	2.41394200	2.55651100	0.09501200
O	0.70597800	0.58963500	1.40339500
O	3.57007300	-0.01074100	1.01623100
O	1.47271000	-1.95207100	0.30741000
O	6.58420700	0.79244300	-0.26929300
O	4.28029500	1.00644000	-1.88107100
O	6.03425900	-1.88173600	0.08038700
O	3.88971200	-1.61627200	-1.70378800
C	2.37740400	3.03233700	1.24803300
C	1.76361200	2.50042900	2.40031200
H	1.88536600	3.02645200	3.33934700
C	1.00291900	1.33857200	2.38473500
C	3.15134300	4.36490500	1.41005100
C	0.45606500	0.83141900	3.73849600
C	3.65481800	-0.83130900	1.98176900
C	2.97843100	-2.02986800	2.17352700
H	3.21516500	-2.61931400	3.05197500
C	1.97357100	-2.50569400	1.30744100
C	4.63846300	-0.37021200	3.07899600
C	1.41750400	-3.91623700	1.63386800
C	6.66787100	2.03659400	-0.51813900
C	5.80644900	2.75299500	-1.37519400
H	6.02895000	3.79555000	-1.54446800
C	4.70847300	2.21309700	-2.04472900
C	7.85562600	2.73584700	0.17637400
C	7.73059400	2.47968800	1.69347700
H	7.72724900	1.40642500	1.90891300
H	6.80351900	2.91310600	2.09335800
H	8.58021700	2.94437200	2.21472700
C	9.14778400	2.07693100	-0.35487200
H	10.02165900	2.51440300	0.14961700
H	9.26099200	2.24176500	-1.43683800
H	9.13748500	0.99636900	-0.16729200
C	7.91181200	4.24990500	-0.07758300
H	8.76317000	4.67357200	0.47413900

H	7.00197800	4.75644300	0.27228400
H	8.05945600	4.48621100	-1.14109400
C	3.99514900	3.01762100	-3.15049800
C	4.64011100	2.54858300	-4.47865900
H	4.50601400	1.46726400	-4.61695600
H	5.71599500	2.77240900	-4.49835600
H	4.16357700	3.06789100	-5.32317200
C	4.17653200	4.53751800	-2.99719300
H	3.58255500	5.04894600	-3.76784600
H	5.22091600	4.84928200	-3.13269100
H	3.82943700	4.88487700	-2.01582500
C	2.48992300	2.70138600	-3.18881700
H	2.31071000	1.63464600	-3.36118600
H	2.02375100	3.25045600	-4.01889400
H	1.99599800	3.01382900	-2.26103800
C	5.83622800	-3.12206100	-0.11803100
C	4.91798600	-3.65275800	-1.04818200
H	4.90721200	-4.72351400	-1.18444700
C	4.03378700	-2.89106100	-1.81639700
C	6.73055500	-4.04646000	0.73379100
C	8.19588300	-3.74600900	0.34844800
H	8.87405500	-4.35194500	0.96683500
H	8.42788000	-2.68569200	0.50512200
H	8.38583800	-3.99177300	-0.70696200
C	6.44096800	-5.54093500	0.52896700
H	6.64322900	-5.86397500	-0.50209800
H	5.40061400	-5.79314400	0.77779200
H	7.09393400	-6.12715600	1.19121900
C	6.50279300	-3.68495400	2.21667000
H	7.15827400	-4.29838500	2.85141200
H	5.46266500	-3.87920500	2.51399200
H	6.72563500	-2.62874700	2.40040700
C	3.16252900	-3.54504900	-2.90825400
C	3.49821400	-5.02561200	-3.14861200
H	3.28827300	-5.64488400	-2.26539600
H	4.55013000	-5.16609000	-3.43413700
H	2.87402800	-5.40458600	-3.97034300
C	1.68104700	-3.43477500	-2.50180900
H	1.04481400	-3.79846800	-3.32072900
H	1.40911200	-2.39918600	-2.28819700
H	1.46122000	-4.02741000	-1.60521900
C	3.40299100	-2.75533500	-4.21466000
H	2.77548800	-3.16915900	-5.01686000
H	4.45441300	-2.82888700	-4.52988000
H	3.15529700	-1.69633200	-4.08694700
F	2.81212200	5.04429100	2.52925800
F	4.48173100	4.12013600	1.47439800
F	2.93415000	5.17854000	0.35943800
F	-0.83677100	0.43807500	3.62427600
F	0.50821100	1.75037500	4.72343100
F	1.16180900	-0.24691200	4.14653300

F	5.86141100	-0.13869200	2.57696300
F	4.76957300	-1.26549800	4.08511200
F	4.19464400	0.78682400	3.62732000
F	2.34691900	-4.86336900	1.34372500
F	0.31443400	-4.19525000	0.92523700
F	1.11172700	-4.04246300	2.94701800
Pb	-1.93632600	-0.16308800	0.59289000
Cu	-5.21354500	0.37478300	0.92482000
O	-2.36184300	-2.46962100	-0.19218800
O	-0.69605300	-0.45622500	-1.47807600
O	-3.58241900	0.07287500	-1.04956600
O	-1.52962000	2.04892600	-0.34774200
O	-6.54618800	-0.87156100	0.30575300
O	-4.20096500	-1.02117700	1.86219100
O	-6.10033700	1.81747400	-0.03153200
O	-3.90766600	1.61812400	1.70146100
C	-2.34232000	-2.91708800	-1.35605700
C	-1.75382500	-2.35089000	-2.50591100
H	-1.88541000	-2.85567300	-3.45523500
C	-0.99872200	-1.18648500	-2.47245100
C	-3.10795100	-4.25158800	-1.54109500
C	-0.45006200	-0.65350100	-3.81452500
C	-3.70882600	0.90405400	-1.99932900
C	-3.06121200	2.12045600	-2.19195000
H	-3.32663800	2.71231300	-3.05961500
C	-2.04936000	2.60267000	-1.34001200
C	-4.69768400	0.43161400	-3.08753300
C	-1.50842500	4.02512700	-1.63181500
C	-6.57809700	-2.12141800	0.53680800
C	-5.66922800	-2.81821800	1.36062500
H	-5.84789300	-3.87118700	1.51681900
C	-4.57913500	-2.24582000	2.01609100
C	-7.76345800	-2.85132400	-0.12967600
C	-7.73803400	-2.52274100	-1.63734600
H	-7.79620500	-1.44199700	-1.80241900
H	-6.81679500	-2.89241100	-2.10797300
H	-8.59416500	-3.00457200	-2.13159300
C	-9.05502700	-2.28434600	0.50107400
H	-9.93314300	-2.74603600	0.02633000
H	-9.09767600	-2.49962900	1.57919700
H	-9.11026600	-1.19779000	0.36097800
C	-7.72931000	-4.37592000	0.05677800
H	-8.57874000	-4.82103100	-0.48085900
H	-6.80844000	-4.81557100	-0.34980700
H	-7.82152700	-4.66666000	1.11295500
C	-3.80926300	-3.03581700	3.09421600
C	-4.39845400	-2.56457600	4.44705500
H	-4.26894300	-1.48131800	4.57248200
H	-5.47024100	-2.79866800	4.51623400
H	-3.87981100	-3.07432700	5.27230300
C	-3.98109600	-4.55840500	2.96032100

H	-3.35370900	-5.05725300	3.71244200
H	-5.01688000	-4.87820200	3.13734000
H	-3.66725900	-4.91147600	1.96965700
C	-2.30660600	-2.70499700	3.06191300
H	-2.12978700	-1.63704800	3.23002100
H	-1.79507800	-3.25144000	3.86626300
H	-1.85618500	-3.00869000	2.10959400
C	-5.94998100	3.06251700	0.18082300
C	-5.03204300	3.61897200	1.09536200
H	-5.06046800	4.68767200	1.24441200
C	-4.09822500	2.88507700	1.83179000
C	-6.90530400	3.95888600	-0.63381200
C	-8.34469500	3.60129600	-0.20179600
H	-9.06550200	4.18573300	-0.79203300
H	-8.54237800	2.53415300	-0.35945100
H	-8.50765800	3.83239900	0.86138600
C	-6.66480400	5.46165000	-0.42623900
H	-6.84771400	5.77030900	0.61277300
H	-5.64217500	5.75398500	-0.70337400
H	-7.35828600	6.02785600	-1.06426900
C	-6.71475200	3.61573700	-2.12601400
H	-7.41197200	4.20970600	-2.73421400
H	-5.69250400	3.84766400	-2.45685400
H	-6.90609100	2.55346700	-2.31056100
C	-3.22641500	3.56159600	2.90952400
C	-3.61144500	5.02637700	3.17171900
H	-3.44592900	5.66025300	2.28950200
H	-4.66061000	5.12475500	3.48380700
H	-2.98221400	5.42137300	3.98198600
C	-1.75109600	3.51201700	2.46888400
H	-1.11070900	3.88593000	3.27982500
H	-1.44626300	2.49084900	2.23134200
H	-1.57591700	4.12709300	1.57796900
C	-3.40848600	2.75194400	4.21325900
H	-2.77811300	3.18094900	5.00512200
H	-4.45448200	2.78487400	4.55254500
H	-3.12597400	1.70382200	4.06993800
F	-2.73145100	-4.92839800	-2.65028300
F	-4.43635400	-4.00861800	-1.64872500
F	-2.92377500	-5.06609000	-0.48590500
F	0.86797100	-0.34724200	-3.70892500
F	-0.57625200	-1.52164500	-4.83765600
F	-1.09294200	0.48407700	-4.15949400
F	-5.87433000	0.06513100	-2.55920700
F	-4.94179500	1.37203000	-4.02905000
F	-4.17988800	-0.64758600	-3.72577400
F	-2.23860900	4.94067400	-0.94281700
F	-0.22834000	4.15152200	-1.24627100
F	-1.58117400	4.35659200	-2.94077900

[Cu(tmhd)<sub>2</sub>]<sub>2</sub> – BS1

Cu,0,-2.9404110042,-1.1153681864,1.5630489601  
O,0,-3.396932744,0.7314754452,1.9516828312  
O,0,-4.5919590095,-1.3311550614,0.5594449107  
O,0,0.9212905735,0.3635182861,-1.8236858854  
O,0,-2.4154254411,-2.9162193343,1.0719928176  
O,0,2.1086643708,2.7192635109,-0.9130531966  
C,0,-4.0610216021,1.4695167366,1.1501283213  
C,0,-4.9137173066,0.9868867956,0.1438398726  
H,0,-5.4317404901,1.7046006835,-0.474202687  
C,0,-5.1688850802,-0.3791614402,-0.0650600911  
C,0,-3.8589436966,2.9798697609,1.3816990759  
H,0,-4.0980170916,2.7186163504,3.5369828901  
C,0,-2.3404891032,3.2391368068,1.4680798645  
H,0,-1.8338654445,2.9550176456,0.5352651995  
H,0,-1.8935834344,2.6581418603,2.281418337  
C,0,-6.2045483,-0.8518606019,-1.1057395392  
C,0,-7.3010303681,-1.6240302946,-0.3412130883  
H,0,-7.8234990986,-0.9653258356,0.366441733  
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C,0,-5.4887765403,-1.8070046095,-2.0840207929  
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C,0,-6.8439522262,0.2976309827,-1.8975274397  
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H,0,-1.0263921052,3.0424935112,-1.9343342234  
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H,0,-2.6408621558,-1.1210659007,-1.5358071451  
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C,0,-2.5174586222,1.3073812195,-2.8340296024  
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H,0,-3.361745179,0.7016799186,-3.1912929334  
C,0,-0.9873779624,-0.5025647259,-3.673758958  
H,0,-1.8563903645,-1.108070419,-3.9663416217  
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C,0,0.8755538679,4.7350991832,-0.9203904255  
C,0,-0.4713266027,5.3520892038,-1.3251340862  
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H,0,-1.3088497755,4.9131474945,-0.768447961  
H,0,-0.455568726,6.4282428072,-1.1057166348  
C,0,2.0101601346,5.4368962236,-1.6959583544

H,0,2.0111003311,6.5110515661,-1.4651076331  
H,0,-3.1574684255,-4.8982106271,-0.1663900873  
H,0,1.8749342733,5.3210289844,-2.780600423  
C,0,1.0946180228,4.9201075963,0.597195781  
H,0,1.0712059232,5.9889813269,0.8507137361  
H,0,0.3088129299,4.4136029597,1.1734645533  
H,0,-1.5992170136,-3.622620563,-1.7277217536  
C,0,-1.2055729622,-3.2956753876,0.9379066832  
O,0,-1.2587985761,-0.8118729128,2.4582665596  
C,0,-0.0837343975,-2.5777587466,1.391239251  
C,0,-1.0122003861,-4.6038742881,0.1418022412  
C,0,-0.1663486291,-1.3863085188,2.1254471794  
H,0,0.8960432344,-2.9741580799,1.1675424691  
C,0,0.1735492961,-5.431954711,0.6693410283  
C,0,-2.2923578257,-5.4531959027,0.2108810554  
C,0,-0.7500122798,-4.1893533257,-1.3252507507  
C,0,1.0936939173,-0.6310048446,2.5911424543  
H,0,0.0594915436,-5.652954321,1.7389554292  
H,0,1.1357235229,-4.9276018123,0.5234351984  
H,0,0.2188742271,-6.386577796,0.1275409966  
H,0,-2.1623193403,-6.36166556,-0.3928281817  
H,0,-2.5108108771,-5.7547859292,1.2440025586  
H,0,-0.6086421939,-5.086194273,-1.9446287966  
H,0,0.1493612668,-3.5658916093,-1.4115596123  
C,0,-4.520729935,3.3307084139,2.7315638426  
C,0,-4.4605475459,3.8523164061,0.2702215886  
C,0,1.0061166554,0.7875624187,1.9871473091  
C,0,2.399058868,-1.2973083372,2.1404059179  
C,0,1.0605734052,-0.5425424043,4.1301939275  
H,0,-5.6052157306,3.1574805086,2.6947283087  
H,0,-4.3505777023,4.3900517335,2.968824881  
H,0,-2.1556605205,4.3070147659,1.6491541521  
H,0,-4.2362715636,4.907683663,0.475918701  
H,0,-5.5523318939,3.7523095866,0.2120584701  
H,0,-4.037203521,3.60548965,-0.7132294978  
H,0,1.9143768554,1.3582623221,2.2211768749  
H,0,0.131752062,1.3220989792,2.3740035517  
H,0,0.9095389956,0.7407293661,0.8938495824  
H,0,2.4667733701,-1.354424586,1.0486216667  
H,0,2.5051043152,-2.3098360792,2.5535294973  
H,0,3.2505352849,-0.7016724989,2.4925851695  
H,0,1.9064651846,0.0624508417,4.4853479233  
H,0,1.1397215557,-1.5406647356,4.5835078234  
H,0,0.1280697504,-0.07862808,4.4712796991  
O,0,4.1336329259,1.2467517749,0.1238690946  
Cu,0,2.6016305709,0.8427771824,-0.9909697546  
C,0,5.1093994752,0.4726304593,0.3962329022  
O,0,3.2472920125,-0.9547516153,-1.3524944759  
C,0,5.2619903691,-0.8349625977,-0.093594183  
C,0,6.1525512753,1.101838469,1.3426382075  
C,0,4.3346022835,-1.4742071175,-0.9300603211

H,0,6.1399282487,-1.3876292353,0.2045583207  
C,0,6.7121933347,2.3564134356,0.6384017189  
C,0,5.419666705,1.520228866,2.6348686195  
C,0,7.3083167925,0.1561400603,1.6985641531  
C,0,4.5452509452,-2.9300270068,-1.3942415708  
H,0,7.2400054888,2.084292003,-0.2864458685  
H,0,5.9015327512,3.0482034118,0.3834523658  
H,0,7.4237365536,2.8709119482,1.2988673348  
H,0,6.1162399344,2.0370297427,3.3090803381  
H,0,4.585284696,2.1923968832,2.4057371953  
H,0,5.0235583621,0.642653917,3.1652612043  
H,0,7.878647949,-0.1443855546,0.8096244053  
H,0,8.0005270732,0.6693025145,2.3795866216  
H,0,6.9512376174,-0.7498418496,2.2063829658  
H,0,2.9834109115,5.0153722696,-1.4215197924  
H,0,2.0636772895,4.5058247795,0.8977276482  
C,0,4.4940423465,-2.944274466,-2.9361436899  
C,0,3.370554211,-3.7587528672,-0.8314298418  
C,0,5.8713020429,-3.5414754395,-0.9208048859  
H,0,3.5510615331,-2.5171076388,-3.2947280145  
H,0,5.3227317037,-2.360508045,-3.3609815997  
H,0,4.5794661194,-3.9759298862,-3.3042401862  
H,0,3.4387078411,-4.7976461554,-1.1819434332  
H,0,3.3881601164,-3.7666419036,0.2676203771  
H,0,2.4139620032,-3.3379615479,-1.1602950054  
H,0,5.9527278953,-4.5691819761,-1.2996530082  
H,0,6.7359559893,-2.9779844689,-1.2959979506  
H,0,5.9325818953,-3.5854736026,0.1747231158

**[Cu(tmhd)<sub>2</sub>]<sub>2</sub> – BS2**

Cu,0,-2.9723875026,-1.0738908173,1.4867338142  
O,0,-3.4219117708,0.7795484454,1.8332804525  
O,0,-4.6060607902,-1.3148304018,0.4586699137  
O,0,0.9946148546,0.3877036171,-1.7659681447  
O,0,-2.4802346602,-2.8979952078,1.0900260977  
O,0,2.1827691292,2.7390453987,-0.8335303909  
C,0,-4.1484982975,1.4990780623,1.0716532909  
C,0,-5.0205132759,0.9969691777,0.0901002105  
H,0,-5.5863626554,1.7038073045,-0.4986814756  
C,0,-5.2300710824,-0.3752053527,-0.135981441  
C,0,-3.9998454728,3.013425913,1.3230643199  
H,0,-4.0703209434,2.7048112581,3.4868377252  
C,0,-2.4919363601,3.341167697,1.3070540849  
H,0,-2.0417135158,3.1005049558,0.333948605  
H,0,-1.9595043359,2.7647689789,2.071899225  
C,0,-6.2696229378,-0.8715995565,-1.1634438663  
C,0,-7.2987407366,-1.7330714594,-0.4001274392  
H,0,-7.840977205,-1.1312988062,0.3441553065  
H,0,-6.8017476574,-2.5602927111,0.1205212194  
H,0,-8.0340445866,-2.1486713601,-1.104755178  
C,0,-5.5250174547,-1.7486724251,-2.1931734822

H,0,-6.2433084633,-2.1792727132,-2.9060326229  
H,0,-4.9897388145,-2.5647920752,-1.693445112  
H,0,-4.7965905751,-1.1541154992,-2.7639983294  
C,0,-6.9994649238,0.2620109983,-1.8988044747  
H,0,-7.5667619834,0.9009943283,-1.2074692691  
H,0,-7.7145141855,-0.1713685104,-2.612935246  
H,0,-6.3043324624,0.8952980984,-2.4683092056  
C,0,0.0012619977,1.1601357664,-1.9754766794  
C,0,-0.0107490642,2.5432272873,-1.7299772006  
H,0,-0.9097050449,3.0919607162,-1.9692821604  
C,0,1.0680775684,3.2536008536,-1.1734989759  
C,0,-1.2539571563,0.4255127109,-2.4898258081  
C,0,-1.7028105986,-0.5007407195,-1.340645658  
H,0,-2.5815945017,-1.0861328835,-1.6384943722  
H,0,-0.8991904632,-1.1889117974,-1.0566503136  
H,0,-1.9720868576,0.0991069269,-0.4602691602  
C,0,-2.4112772763,1.3636131962,-2.8625460791  
H,0,-2.782836584,1.9228098096,-1.9933453187  
H,0,-2.1238133186,2.0772633977,-3.647910238  
H,0,-3.2512552168,0.7653727983,-3.2437636769  
C,0,-0.8594949667,-0.4198423301,-3.7171205631  
H,0,-1.7215849956,-1.0163723092,-4.0498036538  
H,0,-0.5438483618,0.2212790207,-4.5537758782  
H,0,-0.0335484418,-1.0977750535,-3.4727841102  
C,0,0.9708595294,4.7667893812,-0.8857091646  
C,0,-0.3292490206,5.4107790303,-1.390591697  
H,0,-0.4479249969,5.2917983221,-2.4770842011  
H,0,-1.2164778993,4.9956798095,-0.8947145688  
H,0,-0.3047489691,6.4887620247,-1.1744870765  
C,0,2.1739545418,5.4566029499,-1.562641084  
H,0,2.1696874944,6.5305191125,-1.3250123779  
H,0,-3.180594808,-5.2689114348,0.9661119174  
H,0,2.1255318058,5.3493404802,-2.6566072828  
C,0,1.0701008809,4.9385666033,0.64682089  
H,0,1.0420511398,6.0075768601,0.9050464544  
H,0,0.232775018,4.4407646241,1.1555700063  
H,0,-2.5758888422,-4.087015585,-1.2235451775  
C,0,-1.2812882415,-3.3295239738,1.0115961133  
O,0,-1.2757672915,-0.7465822796,2.3547203511  
C,0,-0.1446567949,-2.6286901993,1.4480932268  
C,0,-1.1642162355,-4.7082753596,0.328955316  
C,0,-0.2003684328,-1.3810342262,2.0940783448  
H,0,0.8251140652,-3.0750074229,1.284990241  
C,0,0.246961738,-5.3095517465,0.3971486078  
C,0,-2.1615200634,-5.6701455898,1.0064975235  
C,0,-1.5632848265,-4.50284392,-1.1504291213  
C,0,1.077044842,-0.6496265778,2.5540709373  
H,0,0.5888971167,-5.4277644361,1.4353010909  
H,0,0.9818197542,-4.7003003329,-0.1440210307  
H,0,0.2380715786,-6.3058592187,-0.0683504183  
H,0,-2.1425758335,-6.6446256351,0.4968684851

H,0,-1.8964346684,-5.8320576848,2.0618872616  
H,0,-1.537393305,-5.4660791572,-1.6811500323  
H,0,-0.8692564152,-3.8151912821,-1.6550752487  
C,0,-4.5785162183,3.3078042577,2.7241554149  
C,0,-4.7184269122,3.8812833175,0.2789232203  
C,0,1.0108977556,0.7834389898,1.9835171353  
C,0,2.3673115351,-1.3291786294,2.0765679251  
C,0,1.0604552844,-0.5941678481,4.0962845504  
H,0,-5.6544426557,3.0823348728,2.7626393326  
H,0,-4.4428627391,4.3717611249,2.9688371882  
H,0,-2.3423278116,4.4134455742,1.4994964492  
H,0,-4.5320489442,4.942202845,0.4997337792  
H,0,-5.8066453028,3.7282849736,0.292280899  
H,0,-4.3520669075,3.6822887291,-0.7384902885  
H,0,1.9308273086,1.3316876207,2.227357294  
H,0,0.148586879,1.325384838,2.3881017039  
H,0,0.9069713962,0.7650106238,0.8904842347  
H,0,2.4025805361,-1.4101313686,0.9837021654  
H,0,2.4864353805,-2.3339139648,2.506908741  
H,0,3.2309444028,-0.7292302062,2.391452827  
H,0,1.9270046579,-0.019605874,4.4558842994  
H,0,1.1161111036,-1.603895631,4.5295248223  
H,0,0.144560082,-0.110731491,4.4586169646  
O,0,4.2222129935,1.2524525013,0.1714666998  
Cu,0,2.6869247364,0.869553556,-0.9527397518  
C,0,5.2014702341,0.4768533737,0.422030778  
O,0,3.3503222909,-0.9063190613,-1.3734274268  
C,0,5.3609598644,-0.8168686584,-0.1060210167  
C,0,6.2413461437,1.084678073,1.3879278589  
C,0,4.4377419928,-1.4342336471,-0.9664528661  
H,0,6.2411258247,-1.3748773505,0.1772230667  
C,0,6.776750499,2.3776556114,0.7353575416  
C,0,5.5082002106,1.4353285028,2.7008212827  
C,0,7.4170447902,0.1474666224,1.7005222331  
C,0,4.6616151618,-2.8677278369,-1.4925160339  
H,0,7.3037837197,2.1552766778,-0.2043573286  
H,0,5.9547605968,3.0689125834,0.5145908811  
H,0,7.4853616953,2.873601068,1.4149380618  
H,0,6.2021459506,1.9314737225,3.3949569257  
H,0,4.6634431547,2.1068616551,2.5065400289  
H,0,5.1257823197,0.5293582485,3.1940684103  
H,0,7.9867098586,-0.1117003781,0.7968821748  
H,0,8.1063365531,0.6506373682,2.3939349163  
H,0,7.0831378579,-0.7830226206,2.1813158381  
H,0,3.117900781,5.0209363487,-1.2152142138  
H,0,2.0067001483,4.5089560043,1.0225017283  
C,0,4.6867813912,-2.7991047786,-3.0346862816  
C,0,3.4562704024,-3.7159867578,-1.03341811  
C,0,5.9596284292,-3.516380794,-0.9903490574  
H,0,3.762406147,-2.3505135901,-3.4176099163  
H,0,5.536642302,-2.196681467,-3.3883994004

H,0,4.7889806165,-3.8115577411,-3.4523513452  
H,0,3.539064173,-4.7365060814,-1.4348265763  
H,0,3.417809552,-3.7835730733,0.0636551315  
H,0,2.5176145229,-3.2720907023,-1.3855638816  
H,0,6.0424006149,-4.5304605651,-1.4074647533  
H,0,6.8488615981,-2.9535873356,-1.3078859411  
H,0,5.9761441295,-3.6056720956,0.1051536583

**[Pb(hfac)<sub>2</sub>]<sub>2</sub> – BS1**

Pb,0,-1.3329506461,-0.2597331761,-1.5825914524  
O,0,-2.9426081637,-1.8586921555,-0.8325264213  
O,0,-1.3453391491,0.0215210135,0.7015467404  
O,0,-3.2672948832,0.962812956,-1.3932924441  
O,0,-0.5949099184,1.981150388,-1.1974977048  
C,0,-3.6229648225,-1.834174854,0.2151579233  
C,0,-3.3757768164,-1.0808986824,1.3843240525  
H,0,-4.066298958,-1.1749882518,2.2123385501  
C,0,-2.266054259,-0.2726756447,1.5426767019  
C,0,-4.850608642,-2.765576715,0.1897773326  
C,0,-2.0347419455,0.3481959798,2.9281815232  
C,0,-3.4898852735,2.0264969768,-0.7413363032  
C,0,-2.5691319289,2.9572045468,-0.2573034736  
H,0,-2.9299099765,3.795602155,0.3250337897  
C,0,-1.1940403428,2.8498186605,-0.5124174964  
C,0,-4.983759786,2.2438200732,-0.4503880146  
C,0,-0.2505347996,3.8583778209,0.1690296885  
F,0,-5.5618409105,-2.7148480188,1.3330006413  
F,0,-5.6602576114,-2.4176058796,-0.8218759222  
F,0,-4.4547385184,-4.0345257234,0.000308061  
F,0,-1.0555266189,-0.3386277706,3.5724000992  
F,0,-3.1238909444,0.3314499598,3.705296031  
F,0,-1.6174882531,1.6238219222,2.8152675479  
F,0,-5.6824354742,2.2637283771,-1.5954184965  
F,0,-5.224237182,3.3927170162,0.2088908161  
F,0,-5.4464977708,1.2288246053,0.3066637941  
F,0,0.7701670516,4.1894079892,-0.6301732449  
F,0,0.2704304114,3.2712743153,1.2804339113  
F,0,-0.8717868161,4.9824177527,0.5592478004  
Pb,0,1.3328734645,0.259780285,1.582515785  
O,0,2.9425613194,1.8586505654,0.8323458491  
O,0,1.3452630772,-0.0216295469,-0.7016112673  
O,0,3.2672507518,-0.9627481315,1.3933595475  
O,0,0.5949134843,-1.98115719,1.1975864348  
C,0,3.6229979332,1.8339450872,-0.2152832673  
C,0,3.3758167266,1.0805716662,-1.3843888609  
H,0,4.0663936263,1.1745250636,-2.2123732869  
C,0,2.2660300412,0.2724336461,-1.5427309622  
C,0,4.8507725338,2.7651730121,-0.1898883491  
C,0,2.0347015988,-0.3484865114,-2.928211451  
C,0,3.4898853316,-2.0264706422,0.7414818031  
C,0,2.5691641635,-2.9572176125,0.2574646728

H,0,2.9299732409,-3.7956409855,-0.3248151196  
C,0,1.1940639029,-2.8498338677,0.5125319316  
C,0,4.9837783224,-2.2438022543,0.4506355934  
C,0,0.2505939352,-3.8584725231,-0.1688471132  
F,0,5.5620473737,2.7142946054,-1.3330784655  
F,0,5.660324638,2.4171187611,0.8218152381  
F,0,4.4550821334,4.0341868242,-0.0004858087  
F,0,1.0555295017,0.3383624657,-3.5724676838  
F,0,3.1238621339,-0.3318296181,-3.7053121176  
F,0,1.6173840536,-1.6240873461,-2.8152523532  
F,0,5.6823569299,-2.2637777937,1.5957255341  
F,0,5.2242845931,-3.3926753216,-0.2086743994  
F,0,5.4466019454,-1.2287833516,-0.3063302011  
F,0,-0.7702639022,-4.1892548558,0.6302615627  
F,0,-0.2701468213,-3.2715802996,-1.280464533  
F,0,0.8718184655,-4.9826437469,-0.5587289528

**[Pb(hfac)<sub>2</sub>]<sub>2</sub> – BS2**

Pb,0,-1.395030842,-0.2161613846,-1.5049286987  
O,0,-3.0409810926,-1.8060801958,-0.7970191354  
O,0,-1.408605004,-0.008064791,0.7830836634  
O,0,-3.3143465561,1.0227208524,-1.3391283206  
O,0,-0.6351440872,2.0017665923,-0.9991222087  
C,0,-3.7003567556,-1.8266685194,0.2631145835  
C,0,-3.4413304834,-1.1105573572,1.4550363076  
H,0,-4.1254905277,-1.2257428885,2.2867440942  
C,0,-2.3256784205,-0.3084358577,1.6225135993  
C,0,-4.9169317083,-2.7843610213,0.2333897273  
C,0,-2.089658136,0.3160102316,3.0115711582  
C,0,-3.5564363981,2.111235508,-0.740155972  
C,0,-2.6518967169,3.0527709095,-0.2432408099  
H,0,-3.0349490601,3.9227106151,0.2762219324  
C,0,-1.2650311949,2.9191277482,-0.4132787622  
C,0,-5.0679087808,2.3630183576,-0.549517479  
C,0,-0.3414549849,3.9903020027,0.2099417508  
F,0,-5.6680130287,-2.7106952556,1.3541825054  
F,0,-5.7089742843,-2.4965018413,-0.8141761609  
F,0,-4.4918405124,-4.0573030341,0.1053011372  
F,0,-1.0343496554,-0.2952636253,3.6160061137  
F,0,-3.1440531181,0.211225485,3.8354006933  
F,0,-1.7775531886,1.6240513148,2.8967137438  
F,0,-5.6951151622,2.3803636731,-1.7401869731  
F,0,-5.3344316609,3.5286091475,0.0767720841  
F,0,-5.6044653302,1.3685115974,0.1919571401  
F,0,0.5618761186,4.4250285679,-0.6843780037  
F,0,0.3396456304,3.4349689637,1.2471211636  
F,0,-1.0060401261,5.0592412841,0.6893496156  
Pb,0,1.394994018,0.2163969236,1.5048266841  
O,0,3.0410007397,1.8061427321,0.7966069268  
O,0,1.4085372913,0.0079214403,-0.7831679404  
O,0,3.314336884,-1.0224933224,1.3392356031

O,0,0.6351836132,-2.0016352131,0.9994785448  
C,0,3.7004481156,1.8264063333,-0.263486153  
C,0,3.4414223222,1.1100365376,-1.455255684  
H,0,4.1256477748,1.2249529205,-2.2869471309  
C,0,2.3256872172,0.3080088936,-1.6226194759  
C,0,4.9171135182,2.7839897251,-0.2339213922  
C,0,2.0896440686,-0.3166604899,-3.0115726492  
C,0,3.5564400628,-2.1110785375,0.7403958827  
C,0,2.6519057601,-3.0526693854,0.2435761454  
H,0,3.0349541207,-3.9226515424,-0.2758184659  
C,0,1.2650447535,-2.9190278332,0.4136602616  
C,0,5.0679160303,-2.3628922717,0.5498283506  
C,0,0.3414419785,-3.9902434479,-0.2094462475  
F,0,5.6683051166,2.7099126951,-1.3546133997  
F,0,5.7090173126,2.4963746021,0.8138142076  
F,0,4.4921285869,4.0570122082,-0.1062651998  
F,0,1.0345369901,0.2947574194,-3.6162194423  
F,0,3.1441391593,-0.2122870518,-3.8353268421  
F,0,1.777210712,-1.6246010379,-2.8964960815  
F,0,5.6950657619,-2.3802145352,1.7405295258  
F,0,5.3344436233,-3.5285086093,-0.076412144  
F,0,5.6045319207,-1.3684217776,-0.1916503253  
F,0,-0.5618245985,-4.4249397466,0.6849577898  
F,0,-0.3397361308,-3.4349700627,-1.2466016243  
F,0,1.0060098939,-5.0591986254,-0.6888444231

**[Cu(tmhd)<sub>2</sub>Pb(hfac)<sub>2</sub>] – BS1**

Pb,0,0.0037435294,0.9655173924,-1.6476161894  
Cu,0,-0.1798654061,-2.0437301698,-0.21171789  
O,0,-2.1914052515,1.5871777639,-0.8729918099  
O,0,0.2578857911,3.0791978409,-0.6592158748  
O,0,-0.1128232105,0.3194623537,0.5277476165  
O,0,2.3252769975,1.0625755324,-0.8152647539  
O,0,-1.5634718226,-2.5492397796,1.012653673  
O,0,-1.4342599614,-1.370560115,-1.542930865  
O,0,1.1558135567,-2.6336432797,1.0411281873  
O,0,1.1476251081,-1.6271552204,-1.5739982609  
C,0,-2.4486596412,2.2645469043,0.1556264485  
C,0,-1.6491096333,3.2296417338,0.7853211374  
H,0,-2.0371615348,3.7405240938,1.6567081107  
C,0,-0.3844468301,3.5814602624,0.3062380614  
C,0,-3.8259884043,1.953905047,0.7718991532  
C,0,0.3780924897,4.7178271599,1.0084681042  
C,0,0.6151961075,0.6177033162,1.5332219448  
C,0,1.933819268,1.0343876379,1.5460025418  
H,0,2.4099194174,1.2308104641,2.4990214595  
C,0,2.7079854064,1.1436404499,0.3682228388  
C,0,-0.0912831281,0.4087024159,2.8831203589  
C,0,4.2275011851,1.3174034876,0.5728452066  
C,0,-2.8169962635,-2.3994297541,0.8344285211  
C,0,-3.4104860673,-1.9239209103,-0.3518968898

H,0,-4.4888401589,-1.9093707338,-0.3942827206  
C,0,-2.7219176278,-1.4762341505,-1.4758331006  
C,0,-3.6813684853,-2.8332938064,2.0300695704  
C,0,-3.1634883057,-2.100154564,3.285318072  
H,0,-2.1039553058,-2.3142457652,3.4519438198  
H,0,-3.2809721749,-1.0144925083,3.1818157837  
H,0,-3.7366260921,-2.4289026317,4.1629694708  
C,0,-3.4857896931,-4.3557069363,2.2033435273  
H,0,-4.0502654333,-4.7071000663,3.0778772304  
H,0,-3.8467808014,-4.9036255837,1.3213176411  
H,0,-2.4256390541,-4.5929170054,2.3509190412  
C,0,-5.1744210598,-2.5198335205,1.8488132557  
H,0,-5.7163480391,-2.8075567499,2.7594709002  
H,0,-5.340130763,-1.4476383495,1.6819422372  
H,0,-5.6166510554,-3.0787390269,1.0130285139  
C,0,-3.4799298329,-1.1878555263,-2.7822215178  
C,0,-3.4992371429,-2.5318095585,-3.5524449358  
H,0,-2.4770269643,-2.8819479194,-3.7489409235  
H,0,-4.0280219217,-3.3058838027,-2.9812635395  
H,0,-4.0117761291,-2.4016277857,-4.515693306  
C,0,-4.9224016087,-0.7095227466,-2.5371468734  
H,0,-5.3771208635,-0.4245871088,-3.4953181045  
H,0,-5.5516055649,-1.4964326599,-2.1026388951  
H,0,-4.9455559214,0.1623826796,-1.8728361466  
C,0,-2.7490579893,-0.1380704272,-3.635772899  
H,0,-1.7180105569,-0.446406125,-3.8483278089  
H,0,-3.2692844114,-0.0216651604,-4.595541252  
H,0,-2.7447454134,0.8372075907,-3.1334289316  
C,0,2.4135582589,-2.7061026065,0.8387153784  
C,0,3.0532458461,-2.3658982457,-0.3686730416  
H,0,4.1216873166,-2.5075138851,-0.4236845295  
C,0,2.4104583157,-1.8787947065,-1.5075905087  
C,0,3.2232440266,-3.2026337614,2.0492324405  
C,0,2.5641955053,-4.4983698515,2.5649682698  
H,0,3.0858064038,-4.8471505303,3.4664433667  
H,0,1.5105215221,-4.3259613153,2.8091366889  
H,0,2.6188690927,-5.2950735568,1.8094312319  
C,0,4.7013056978,-3.4708754316,1.726683948  
H,0,4.8173039281,-4.2237837801,0.935352298  
H,0,5.2232691097,-2.5551713638,1.4200510611  
H,0,5.2027851622,-3.8517594441,2.6262382475  
C,0,3.1403820098,-2.1097140867,3.1386903956  
H,0,3.6674792066,-2.4494665491,4.0407517078  
H,0,3.615575161,-1.1829645899,2.7933014881  
H,0,2.0995700185,-1.8962155365,3.4002450436  
C,0,3.1893123692,-1.7075629084,-2.8225013615  
C,0,4.6766821876,-1.3811552637,-2.5961826102  
H,0,4.8019604791,-0.4861692401,-1.9747481746  
H,0,5.2187079954,-2.2114124198,-2.1266450736  
H,0,5.1549684567,-1.1904067738,-3.5661817711  
C,0,2.5681635536,-0.6020878665,-3.6931872099

H,0,3.0857256482,-0.5649185411,-4.6607129293  
H,0,1.5058354669,-0.7958547792,-3.88345982  
H,0,2.6798479515,0.3784557478,-3.2132185652  
C,0,3.0596783435,-3.0627518403,-3.5609674288  
H,0,3.5781774448,-3.0108312983,-4.5283265714  
H,0,3.5049326656,-3.8765022744,-2.973731782  
H,0,2.0046822385,-3.3047190135,-3.7463955356  
F,0,-4.1813289674,2.8220261844,1.7368602794  
F,0,-3.8204680521,0.7181784672,1.3134535221  
F,0,-4.7821031653,1.9802264693,-0.1772622393  
F,0,0.6172504091,5.7178460277,0.1421122364  
F,0,-0.291731911,5.2295835872,2.0596418519  
F,0,1.5645848925,4.2653924094,1.4587392222  
F,0,-0.0615485451,-0.8919992934,3.2364005372  
F,0,0.4937687037,1.1141312902,3.8710785746  
F,0,-1.3796900977,0.7842642649,2.8141356081  
F,0,4.7760108356,0.1317382617,0.9366722693  
F,0,4.8348399446,1.7198920521,-0.5488102448  
F,0,4.4959813386,2.2056184825,1.5475143407

**[Cu(tmhd)<sub>2</sub>Pb(hfac)<sub>2</sub>] – BS2**

Pb,0,0.0236755831,0.9448597934,-1.6058987322  
Cu,0,-0.1855753063,-2.0809868164,-0.1965517592  
O,0,-2.1601414417,1.631980649,-0.8354104781  
O,0,0.3268607541,3.0831594066,-0.6592345127  
O,0,-0.0746224135,0.3173400606,0.5819081394  
O,0,2.3664849635,1.049266639,-0.7920104979  
O,0,-1.567315293,-2.6056290706,1.0170731584  
O,0,-1.4468491768,-1.3531778179,-1.4944732808  
O,0,1.1513139538,-2.6787339817,1.0486199653  
O,0,1.1426827785,-1.6363906343,-1.5476829933  
C,0,-2.4210488257,2.3878258063,0.1348806975  
C,0,-1.6102577202,3.3712684541,0.7226374911  
H,0,-2.0047259557,3.9451331436,1.5519160339  
C,0,-0.3271671031,3.6648398818,0.2488221761  
C,0,-3.8461775361,2.1920450735,0.7027420159  
C,0,0.4313804415,4.8575421452,0.8735137019  
C,0,0.6608928036,0.6377885122,1.5739895647  
C,0,1.9756601009,1.071280489,1.5712734649  
H,0,2.4518971329,1.2988062828,2.5182952725  
C,0,2.7418729851,1.1868742406,0.3872615585  
C,0,-0.0461703575,0.4617649752,2.9343808726  
C,0,4.2528742806,1.4711213303,0.5877668572  
C,0,-2.8238658599,-2.5070186869,0.8243177262  
C,0,-3.4196774737,-2.0097640593,-0.3518874738  
H,0,-4.4981478008,-2.0342822454,-0.4130417822  
C,0,-2.731347711,-1.4865022225,-1.4456044061  
C,0,-3.6792324351,-2.9950495407,2.0056424678  
C,0,-3.3347536053,-2.1004938,3.2177543905  
H,0,-2.2672803105,-2.1599863648,3.4540528994  
H,0,-3.5851119989,-1.0493423823,3.0175385005

H,0,-3.9114264241,-2.431065524,4.0939214203  
C,0,-3.2772631539,-4.4546194133,2.3091972646  
H,0,-3.8286724791,-4.8161457422,3.1892055426  
H,0,-3.5164164606,-5.1153938636,1.4623398312  
H,0,-2.202362902,-4.527068153,2.5123132465  
C,0,-5.1912073531,-2.9263634947,1.7425927778  
H,0,-5.7271132355,-3.2894378406,2.6310251756  
H,0,-5.52715081,-1.8978263113,1.5507587236  
H,0,-5.4914199487,-3.5584784448,0.8943156533  
C,0,-3.498236264,-1.1396177856,-2.7348158926  
C,0,-3.7253659198,-2.4849812346,-3.4691031251  
H,0,-2.7680625088,-2.9762069484,-3.6945500283  
H,0,-4.3310417974,-3.1718387117,-2.8630411843  
H,0,-4.2515662519,-2.3046584335,-4.4181871231  
C,0,-4.8545894266,-0.469422435,-2.4436248433  
H,0,-5.3266331711,-0.1808823135,-3.3939456296  
H,0,-5.551844997,-1.1402734731,-1.9255580518  
H,0,-4.7261096909,0.4342878019,-1.8362416255  
C,0,-2.6796814764,-0.2110922754,-3.6464582715  
H,0,-1.69140768,-0.6320667067,-3.869892149  
H,0,-3.2128676941,-0.0731877873,-4.5974266783  
H,0,-2.560891051,0.7797139,-3.1884895748  
C,0,2.4086580249,-2.7518320779,0.846379984  
C,0,3.0486731953,-2.4006804198,-0.3589359637  
H,0,4.1170750741,-2.5475388877,-0.4187691477  
C,0,2.4034360301,-1.9009364546,-1.4922535451  
C,0,3.2104597302,-3.278024168,2.049723605  
C,0,2.6080075064,-4.640543984,2.4558179585  
H,0,3.1231868589,-5.0224295647,3.3489901087  
H,0,1.5393104289,-4.5421043998,2.6789305426  
H,0,2.7278690206,-5.3810194078,1.6508062701  
C,0,4.7105775512,-3.4479403871,1.7646622215  
H,0,4.8959894232,-4.1657414195,0.9526551409  
H,0,5.190343955,-2.493743112,1.5068136081  
H,0,5.2060187877,-3.8337996601,2.6668632835  
C,0,3.0272172514,-2.2687607767,3.2052491828  
H,0,3.5539256575,-2.6327040164,4.0992442327  
H,0,3.4446218529,-1.2873802225,2.9397790057  
H,0,1.9670348348,-2.1433141797,3.448762896  
C,0,3.1757754643,-1.7335772401,-2.8125444036  
C,0,4.6541532604,-1.3626663371,-2.5942576998  
H,0,4.7513897809,-0.4478371253,-1.9961040547  
H,0,5.2204699783,-2.1643235931,-2.1026049507  
H,0,5.1285605437,-1.1824522312,-3.5694846993  
C,0,2.5266934483,-0.6604960735,-3.7035693193  
H,0,3.0402922325,-0.6341530165,-4.6747433729  
H,0,1.4670558804,-0.8775202645,-3.8856734769  
H,0,2.6226452016,0.3344826757,-3.2490099716  
C,0,3.0823422581,-3.1046834859,-3.5280378524  
H,0,3.5985769929,-3.0524890457,-4.4979575461  
H,0,3.5516207628,-3.8974463812,-2.9294665983

H,0,2.0342989538,-3.3811335965,-3.7091825559  
F,0,-4.110613682,2.9691308526,1.7747929546  
F,0,-4.0334648253,0.9086681524,1.0726754098  
F,0,-4.7679325505,2.4825203837,-0.2458340623  
F,0,0.6032888072,5.8312505301,-0.046661964  
F,0,-0.210259662,5.4029730995,1.9305857239  
F,0,1.6526439502,4.4692143006,1.2962119229  
F,0,-0.1307093724,-0.8428211461,3.262720621  
F,0,0.6028603112,1.0931163029,3.9393971415  
F,0,-1.3002882802,0.9546543635,2.8882342894  
F,0,4.8775390763,0.3479482335,1.032206314  
F,0,4.8471603015,1.8438894754,-0.5534207123  
F,0,4.4621293278,2.4376374051,1.5078125334

**[Cu(hfac)(tmhd)] – BS1**

Cu,0,0.0453040192,0.0000124916,0.0001051126  
O,0,-1.3202341343,-1.3973739991,0.0002093824  
O,0,-1.3202128571,1.397419749,0.0001562464  
O,0,1.3458107023,-1.3826497625,0.0000640833  
O,0,1.3458319669,1.3826545078,-0.0000056859  
C,0,-2.5709922148,-1.2141865274,0.0002789355  
C,0,-3.2621400447,0.0000376642,0.0002963657  
H,0,-4.3440609445,0.0000459162,0.0003597322  
C,0,-2.5709737376,1.2142513274,0.000232999  
C,0,-3.368449226,-2.5278317619,0.0003502477  
C,0,-3.3684107461,2.5279087182,0.0002545778  
C,0,2.620012462,-1.2373306548,0.00002221  
C,0,3.2788890403,-0.0000125153,-0.0000102972  
H,0,4.3584188942,-0.0000207054,-0.0000327131  
C,0,2.6200315886,1.237315631,-0.0000417851  
C,0,3.3899196797,-2.5665878503,-0.0000510037  
C,0,3.3899598913,2.5665606592,-0.0001642513  
F,0,-3.0596060403,3.2524356437,1.0890127157  
F,0,-3.0597346486,3.2523933166,-1.0885682857  
F,0,-4.6995649454,2.3221408865,0.0003371759  
F,0,-4.6996002874,-2.3220436639,0.0004258873  
F,0,-3.0596549337,-3.2523226962,1.0891352544  
F,0,-3.0597847849,-3.252361752,-1.0884457484  
C,0,2.9648612365,-3.3493744687,-1.2618290118  
H,0,1.879934762,-3.5009381099,-1.2762469814  
H,0,3.2540594173,-2.8103621175,-2.1749662997  
H,0,3.4589444235,-4.3302631091,-1.2741111062  
C,0,2.96472465,-3.3496616874,1.261494661  
H,0,3.2538553456,-2.8108780337,2.1747891506  
H,0,1.8797935752,-3.5011959171,1.2757864625  
H,0,3.4587801977,-4.330566006,1.273587414  
C,0,4.9149139598,-2.3875938052,0.0000537608  
H,0,5.26326522,-1.8491368987,-0.891436575  
H,0,5.2631531283,-1.8492767575,0.8916726815  
H,0,5.3942274546,-3.3754096577,0.0000031212  
C,0,2.9648678131,3.3493466917,-1.2619293998

H,0,3.2540312016,2.8103293134,-2.1750748707  
H,0,1.87994255,3.5009205802,-1.2763134887  
H,0,3.458960288,4.3302303705,-1.2742303034  
C,0,2.9648245557,3.3496495207,1.2613939434  
H,0,1.8798972667,3.5012092101,1.2757192875  
H,0,3.2539724267,2.8108619502,2.1746804989  
H,0,3.4589030542,4.3305426649,1.2734670711  
C,0,4.9149510732,2.3875414589,-0.0001157693  
H,0,5.263216383,1.8492292778,0.8914958528  
H,0,5.2632579676,1.8490679785,-0.8916134418  
H,0,5.3942810206,3.3753493594,-0.0001960231

**[Cu(hfac)(tmhd)] – BS2**

Cu,0,0.052211076,0.0000123482,0.000090733  
O,0,-1.324590988,-1.3959566119,0.0001806408  
O,0,-1.3245696803,1.3960025538,0.0001298814  
O,0,1.3500019991,-1.3826401026,0.0000578639  
O,0,1.3500232987,1.3826445553,-0.0000012738  
C,0,-2.5734468713,-1.2147965445,0.000237491  
C,0,-3.2684133649,0.0000378044,0.0002492538  
H,0,-4.3511453294,0.0000460816,0.0003014227  
C,0,-2.5734283308,1.2148615555,0.0001933585  
C,0,-3.3742511825,-2.5343584324,0.0002987717  
C,0,-3.3742125096,2.5344356769,0.0002065215  
C,0,2.6234737945,-1.2389508783,0.0000110075  
C,0,3.2833383299,-0.0000126343,-0.0000262336  
H,0,4.3632709053,-0.0000209266,-0.000053539  
C,0,2.623492866,1.2389356304,-0.0000429697  
C,0,3.3921209691,-2.5700832249,-0.0000494714  
C,0,3.392160963,2.5700557885,-0.0001406371  
F,0,-3.0698681986,3.2656184001,1.0910999609  
F,0,-3.0699740303,3.2655756499,-1.0907452455  
F,0,-4.7106153955,2.3343878939,0.0002752546  
F,0,-4.7106510148,-2.3342902596,0.0003625991  
F,0,-3.0699162499,-3.2655072815,1.0912174748  
F,0,-3.0700256621,-3.2655415677,-1.0906277372  
C,0,2.9664312328,-3.353556822,-1.2620567755  
H,0,1.8812293265,-3.508682884,-1.2770909555  
H,0,3.254059376,-2.8149324599,-2.1771246071  
H,0,3.4632922869,-4.3343344738,-1.2738099415  
C,0,2.966488625,-3.3536789758,1.2618972007  
H,0,3.2541516027,-2.8151421007,2.1770064543  
H,0,1.881288247,-3.5088062091,1.2769729017  
H,0,3.4633542103,-4.3344549505,1.2735380013  
C,0,4.9181483113,-2.3960838728,-0.0000756874  
H,0,5.2707814949,-1.8599172345,-0.8925655522  
H,0,5.270805202,-1.8599038245,0.892397551  
H,0,5.3933731674,-3.3871772225,-0.0000785271  
C,0,2.9664936172,3.3535026265,-1.2621708837  
H,0,3.2541212,2.8148505656,-2.1772226469  
H,0,1.8812943726,3.5086447916,-1.2772184181

H,0,3.4633698824,4.3342723705,-1.2739450761  
C,0,2.9665314551,3.3536929327,1.2617822487  
H,0,1.8813329373,3.5088354695,1.2768454506  
H,0,3.2541811945,2.8151779774,2.176908402  
H,0,3.4634101921,4.3344626428,1.2733979473  
C,0,4.9181852425,2.3960313745,-0.0001502187  
H,0,5.2708297926,1.8598932189,0.892352973  
H,0,5.2708127211,1.8598111265,-0.8926101801  
H,0,5.3934265862,3.3871168896,-0.0002029985

**[Pb(hfac)(tmhd)] – BS1**

Pb,0,11.1711735102,11.6651615001,1.8248457024  
O,0,9.1785128929,13.0551839291,1.4822768427  
O,0,9.7186616222,10.357186433,0.6632557602  
O,0,9.9842373714,11.3211095814,3.6242219006  
O,0,11.8300885069,9.5765164901,2.3562105936  
C,0,8.0017047379,12.6286506295,1.426742411  
C,0,7.5653894348,11.338179846,1.0661580534  
H,0,6.5031106654,11.1312730297,1.0506348865  
C,0,8.4493483299,10.3316157534,0.6942400393  
C,0,6.9313093553,13.6832075601,1.7699502403  
C,0,7.8718225619,8.9644573165,0.2918793239  
C,0,9.5622539239,10.2070667508,4.1250033601  
C,0,10.004645179,8.938605515,3.7358723513  
H,0,9.4937837692,8.0891535595,4.1624651687  
C,0,11.0918675355,8.6698710031,2.881592457  
C,0,8.5181562128,10.3847325972,5.2364973318  
C,0,11.5008589078,7.2289877861,2.5458382603  
F,0,5.6947835536,13.1549901379,1.8762645907  
F,0,7.2241151921,14.2799449423,2.9386560307  
F,0,6.8970362907,14.6301761006,0.8150161932  
F,0,8.4728264508,8.4983587176,-0.8138710543  
F,0,6.5457164396,9.0034848243,0.0631953403  
F,0,8.0876515293,8.0704974676,1.2841195389  
C,0,7.3780086187,11.281457205,4.7111865371  
H,0,7.7595185491,12.253280019,4.3833549431  
H,0,6.8603389897,10.807129562,3.8668383486  
H,0,6.6432977432,11.4494568452,5.5100085297  
C,0,9.231381425,11.0976450579,6.4084270962  
H,0,8.516449534,11.2806788701,7.2219246246  
H,0,10.0501393047,10.4809875102,6.8043113963  
H,0,9.6446809327,12.0587773247,6.0828028152  
C,0,7.9266041336,9.057263832,5.7343672146  
H,0,8.693233424,8.404648352,6.1721214067  
H,0,7.1817829916,9.2636705169,6.5140714301  
H,0,7.4217079772,8.5097534891,4.9270495809  
C,0,11.517876018,7.0969595011,1.0064355074  
H,0,10.5166217147,7.2512798325,0.5860774166  
H,0,12.1947884405,7.8329597665,0.560182978  
H,0,11.8583732933,6.0903005377,0.7281435972  
C,0,12.9248310326,7.0078288198,3.1008274441

H,0,12.9380739789,7.0893350699,4.1967582425  
H,0,13.2783584324,6.0039185448,2.8291997512  
H,0,13.6205478496,7.7476412938,2.6893918761  
C,0,10.5516469213,6.1700949187,3.1268396222  
H,0,10.8889629983,5.1724786288,2.8159908159  
H,0,10.537983031,6.1861142949,4.2249997898  
H,0,9.5261794028,6.3064420366,2.7598186534

**[Pb(hfac)(tmhd)] – BS2**

Pb,0,11.1385544414,11.6194793163,1.853765431  
O,0,9.181446613,13.1083792354,1.5571883282  
O,0,9.6205832068,10.3942438581,0.681198727  
O,0,9.953213859,11.2414605982,3.6402555926  
O,0,11.782172497,9.5149723959,2.3208162497  
C,0,7.9926952925,12.7564540228,1.3982275288  
C,0,7.5065045408,11.5018545334,0.9721581994  
H,0,6.4370501901,11.3602958576,0.8772611697  
C,0,8.3545151435,10.452783015,0.6289783295  
C,0,6.9590064228,13.8741654731,1.684021194  
C,0,7.725779416,9.1392145185,0.1183020893  
C,0,9.5611450148,10.1264814426,4.1606490707  
C,0,10.0328954542,8.8612866903,3.79081198  
H,0,9.5622495733,8.0079297524,4.2557396924  
C,0,11.1025811118,8.6030528059,2.9091053759  
C,0,8.5124327488,10.3019876505,5.2690697141  
C,0,11.5600034562,7.1682050122,2.6072833794  
F,0,5.6789246982,13.4364608029,1.6523587052  
F,0,7.1724731815,14.4136084645,2.9008093868  
F,0,7.074528559,14.8593231571,0.7673365019  
F,0,8.2629855634,8.7801531763,-1.064038361  
F,0,6.3866927637,9.2148640115,-0.0454700418  
F,0,7.9672640679,8.1391205633,0.9997009238  
C,0,7.3387827903,11.127744807,4.6990312304  
H,0,7.6863582246,12.100484681,4.3342977794  
H,0,6.8489264401,10.5988131394,3.8691069296  
H,0,6.5893454158,11.2979064355,5.4850139613  
C,0,9.187895221,11.0935705745,6.4127679608  
H,0,8.4601001046,11.2782963045,7.2159738452  
H,0,10.0311463795,10.5300839418,6.8386722635  
H,0,9.5612092473,12.0590224319,6.0504454621  
C,0,7.9732257059,8.9741440423,5.8227986552  
H,0,8.765169147,8.3679406138,6.2845221872  
H,0,7.2236923873,9.1851630378,6.5985043157  
H,0,7.4835743676,8.3741308667,5.0426019837  
C,0,11.4622765515,6.9678467007,1.0775462196  
H,0,10.4244636917,7.0653248622,0.7317225645  
H,0,12.0715013468,7.7093421867,0.5476033053  
H,0,11.8213686871,5.962480298,0.8140560234  
C,0,13.0334122141,7.0416614492,3.0536348456  
H,0,13.1304570483,7.1779556182,4.1410663285  
H,0,13.4135619629,6.04145055,2.8002584647

H,0,13.6580154287,7.7913992508,2.553327414  
C,0,10.7216350319,6.0889355692,3.3093555107  
H,0,11.1016071626,5.096734726,3.0274930565  
H,0,10.7824609978,6.1664587024,4.4043902973  
H,0,9.6645573398,6.1358461564,3.0124751693