Binuclear Copper(I) Borohydride Complex Containing Bridging Bis(diphenylphosphino) methane ligands: Polymorphic Structures of $[(\mu_2\text{-dppm})_2Cu_2(\eta^2\text{-}BH_4)^2]$ Dichloromethane Solvate

Natalia V. Belkova [1], Igor E. Golub [1,2], Evgenii I. Gutsul [1], Konstantin A. Lyssenko[1], Alexander S. Peregudov [1], Viktor D. Makhaev [3], Oleg A. Filippov [1], Lina M. Epstein [1], Andrea Rossin [4], Maurizio Peruzzini [4] and Elena S. Shubina [1,*]

[1] A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences (INEOS RAS), 28 Vavilova St, 119991 Moscow, Russia.; nataliabelk@ineos.ac.ru
[2] Inorganic Chemistry Department, Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklay St, 117198 Moscow, Russia; seraph347@gmail.com
[3] Institute of Problems of Chemical Physics, Russian Academy of Sciences (IPCP RAS), 1 Academician Semenov Avenue, 142432Chernogolovka, Moscow Oblast, Russia; vim@icp.ac.ru
[4] Istituto di Chimica dei Composti Organometallici Consiglio Nazionale delle Ricerche (ICCOM CNR), via Madonna del Piano 10, 50019 Sesto Fiorentino (Florence), Italy; maurizio.peruzzini@iccom.cnr.it
* Correspondence: shu@ineos.ac.ru; Tel.: +7-495-135-5085

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Lists of abbreviations

1,4-bcpvb = 1,4-bis(2-(4-cyanophenyl) vinyl)benzene-N,N'

2,2-biPy = 2,2-bipyridine

2,2-biPy-tzl= 2,2'-bipyridin-6-yl)-tetrazolato

2-Py = 2-pyridine

2-Py-CH$_2$-6-Cou = (2-pyridyl)methyliden]-6-coumarin

2-pyO = 2-hydroxypyridine

2-sba = 2-sulfobenzoic acid

3,5-(6-2,2-biPy)Pzl = 3,5-bis{6-(2,2'-dipyridyl)} pyrazole

4,4-biPy = 4,4-bipyridine

4-Py = 4-pyridine

Boc = tert-butoxycarbonyl

BOC-5,6-anh-nc = 2-Boc-5,6-anhydride-naphthylcarboxylate

bpdcn = biphenyl-4,4'-dicarbonitrile-N,N'

Bphen = bathophenanthroline (4,7-diphenyl-1,10-phenanthroline)

BrbiPyBr = 5,5′-dibromo-2,2′-bipyridine

BrPhenBr = 3,8-dibromo-1,10-phenanthroline

Bzm = benzimidazole

cca = 2-(9H-carbazol-9-yl) acetic acid

cyclam = 1,4,8,11-tetraazacyclotetradecane

Dmphen = 2,9-dimethyl-1,10-phenantroline

dppb = 1,4-bis(diphenylphosphino)butane

dppe = 1,2-bis(diphenylphosphino)ethane

dppf = 1,1-bis(diphenylphosphino)ferrocene

dpph = 1,6-bis(diphenylphosphino)hexane

dppm = bis(diphenylphosphino)methane

eddbn = 4,4'-ethene-1,2-diyldibenzonitrile-N,N'

edt = ethanedithiolate

EtP$_3$ = 1,1,1-tris(diphenylphosphino)-ethyl)ethane

Fc = ferrocene

fptzH = 5-trifluoromethyl-3-(2′-pyridyl)-1H-1,2,4-triazole

Hbmp = 2-(2-benzimidazolyl)-6-methylpyridine

L$_{NN}$ = 1,2-bis[2-(4-methyl-7-acetylamino-1,8-naphthyridine)]ethylene

m-fmptzH = 5-trifluoromethyl-3-(5′-methyl-2′-pyridyl)-1H-1,2,4-triazole

mnt = cis-1,2-dicyanoethylene-1,2-dithiolate

mpyO = 6-metylpyridin-2-olate

N^C^N = 1-methyl-3,5-di(2-pyridyl)benzene

N^C^N = 1-methyl-3,5-di(2-pyridyl)benzene

N^N = 2-(2-tert-butyl-tetrazol-5-yl)pyridine

N^N^OH = 2,4-dimethyl-7-hydroxyl-1,8-naphthyridine

NMP = 2-(4-Dimethylaminophenyl)imidazo (4,5-f)(1, 10)phenanthroline

NP$_3$ = tris(2-(diphenylphosphino)ethyl)amine

NPN = bis(2-pyridyl)phosphole

NPP = 2-pyridylbis(diphenylphosphino)methane

n-PyCO$_2$ = n-pyridylcarboxylate

o-bmptzH = 5-tert-butyl-3-(6′-methyl-2′-pyridyl)-1H-1,2,4-triazole

OCCL = 2-cyano-3-(4-(diphenylamino)phenyl) acrylic acid)

o-fmptzH = 5-trifluoromethyl-3-(6′-methyl-2′-pyridyl)-1H-1,2,4-triazole

paa or N^N-N^N = pyridine-2-carbaldehyde azine

p-fmptzH = 5-trifluoromethyl-3-(4′-methyl-2′-pyridyl)-1H-1,2,4-triazole

phen = phenantroline

pht = phthalimide

pmk = bis(2-pyridylmethyl) ketazine

PPDMe = [3,6-bis(3,5-dimethylpyrazol-1-yl)pyridazine]

Pydz = pyridazine

pymS = pyrimidine-2-thionato

pyz = pyrazine

TCNQ = 7,7,8,8-tetracyanoquinodimethane

tddeddbn = thiene-2,5-diyldiethene-2,1-diyl)dibenzonitrile-N,N'

tmsc = thiosemicarbazide ligand

triphos = 1,1,1-tris(diphenylphosphinomethyl) ethane

tsac = thiosaccharin

ttfa = thenoyltrifluoroacetone

ttfac = 2-thenoyltrifluoroacetone

Figure S1. ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 298K, ppm) of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$.

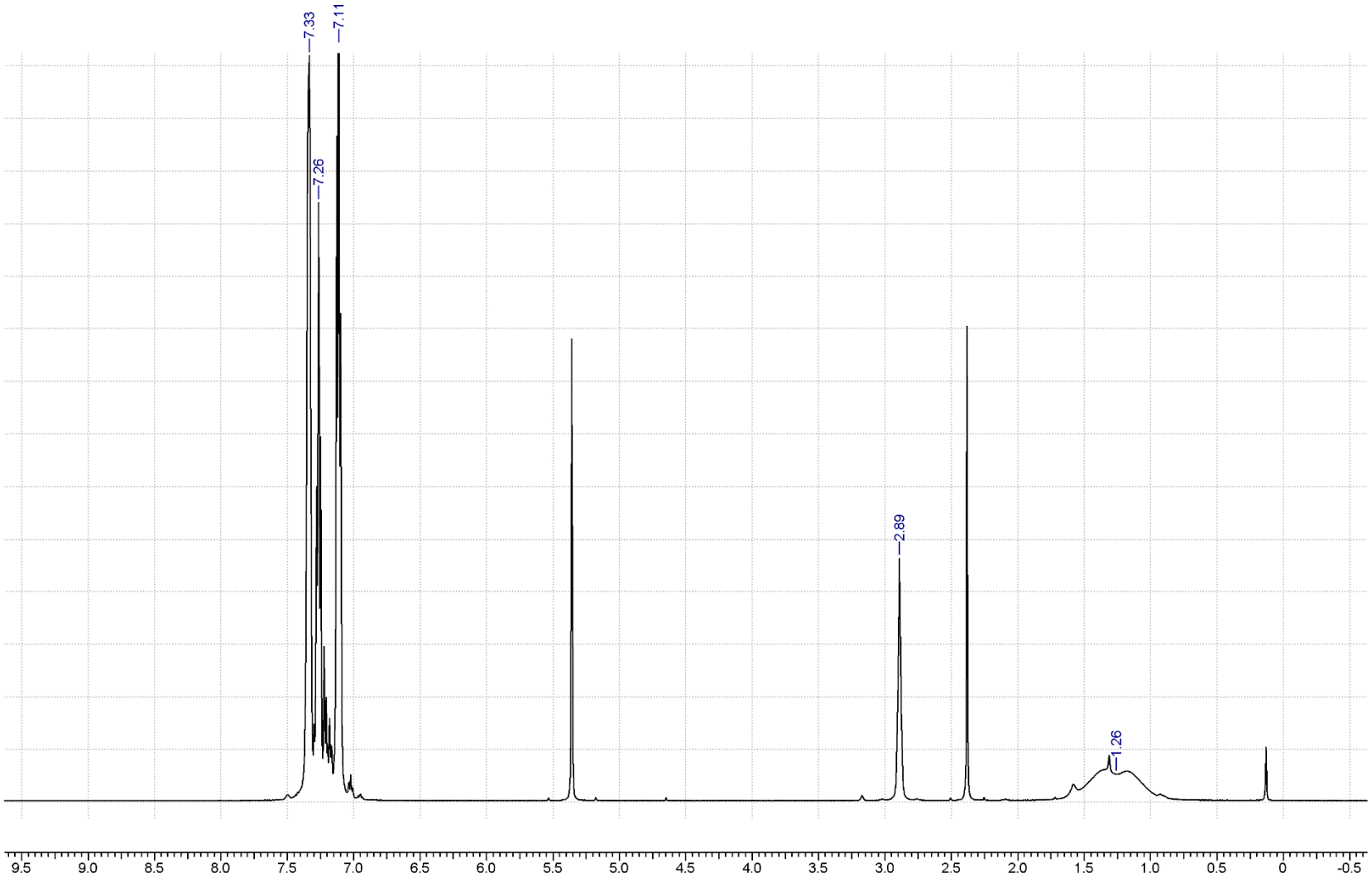


Figure S2. $^{11}B\{^{1}H\}$ NMR spectra (160 MHz, CD_2Cl_2, 298K, ppm) of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$.

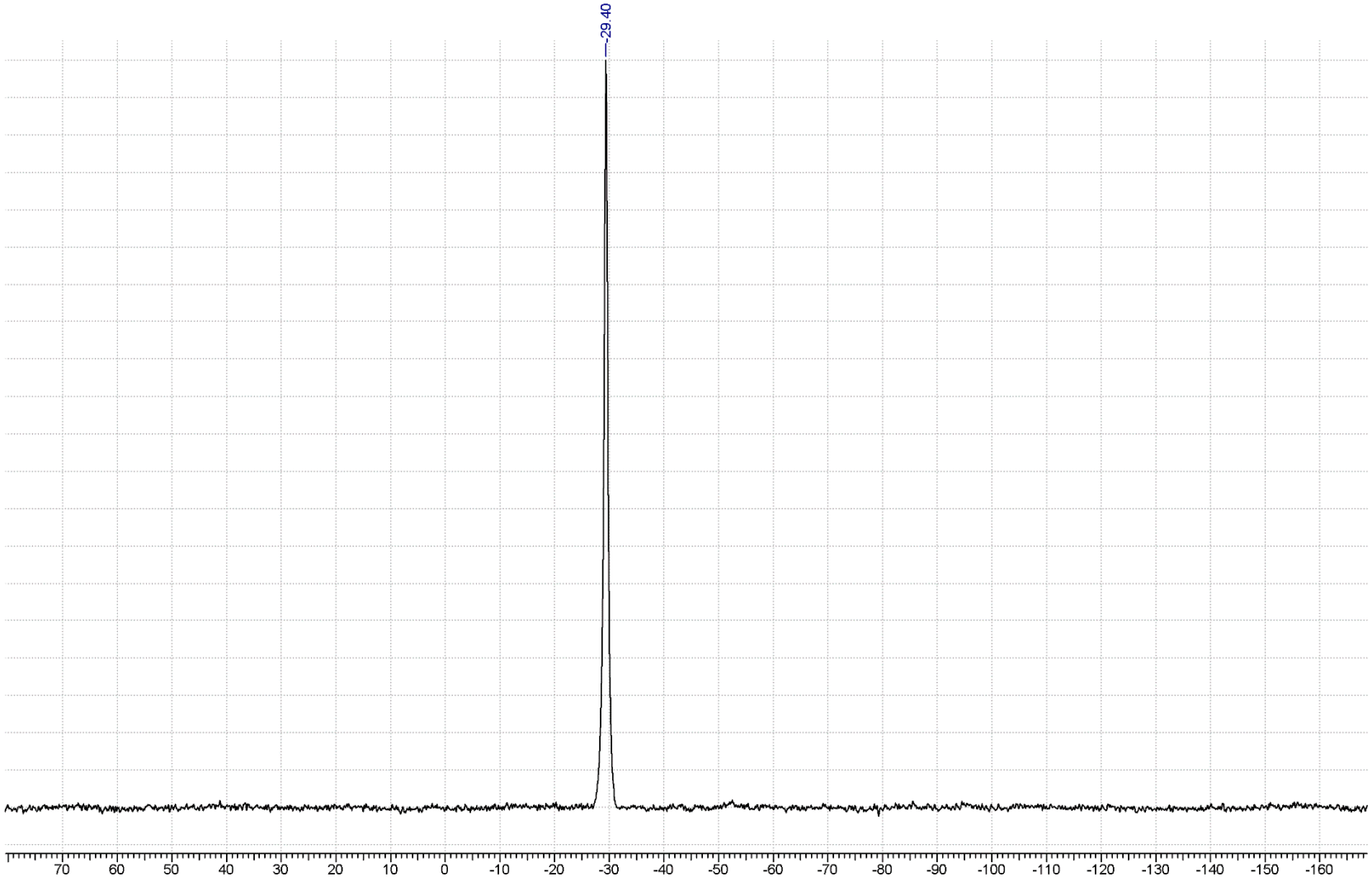


Figure S3. $^{31}P\{^{1}H\}$ NMR spectra (202 MHz, CD_2Cl_2, 298K, ppm) of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$.

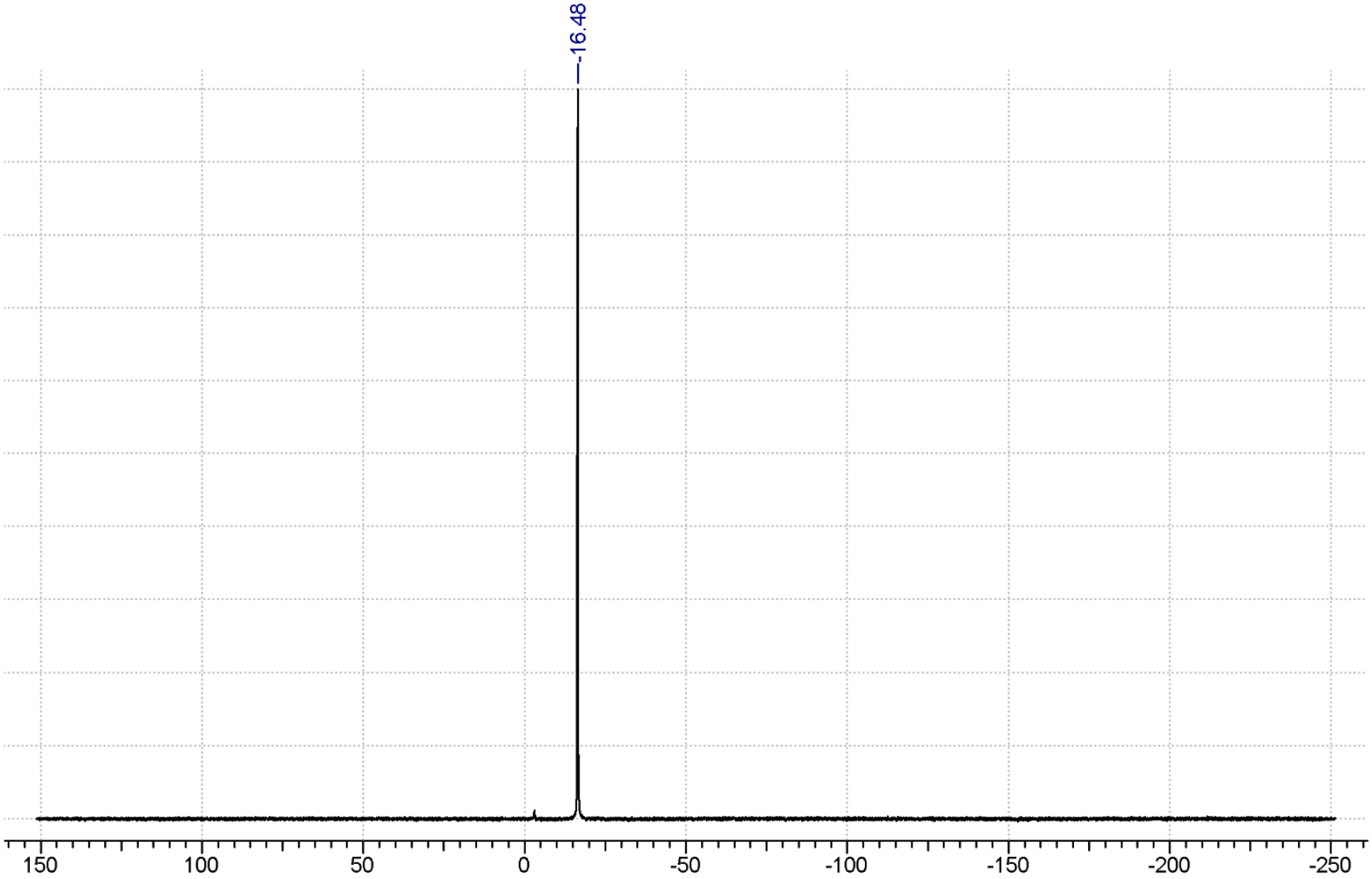


Figure S4. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, CD_2Cl_2, 298K, ppm) of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$.

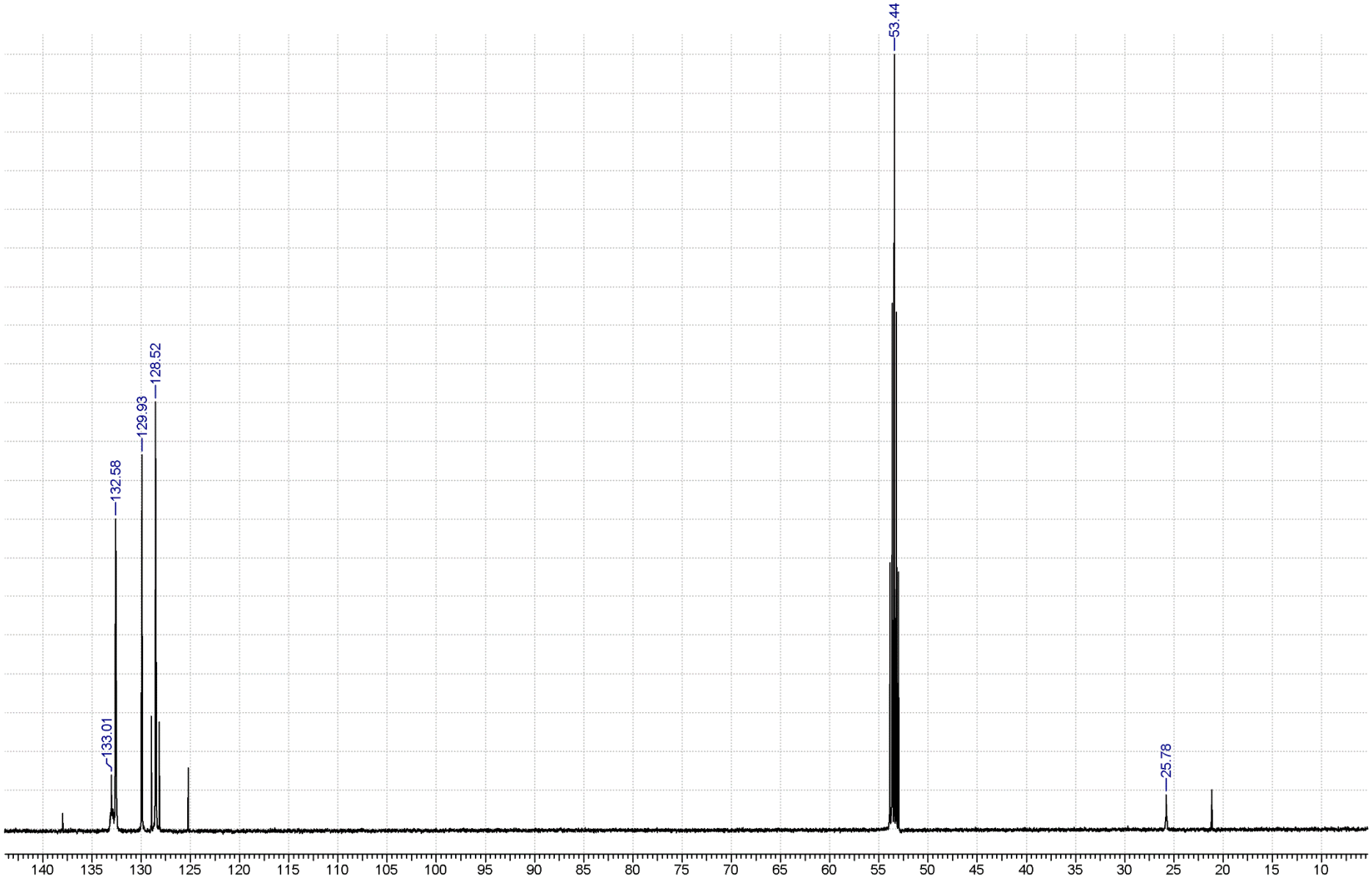
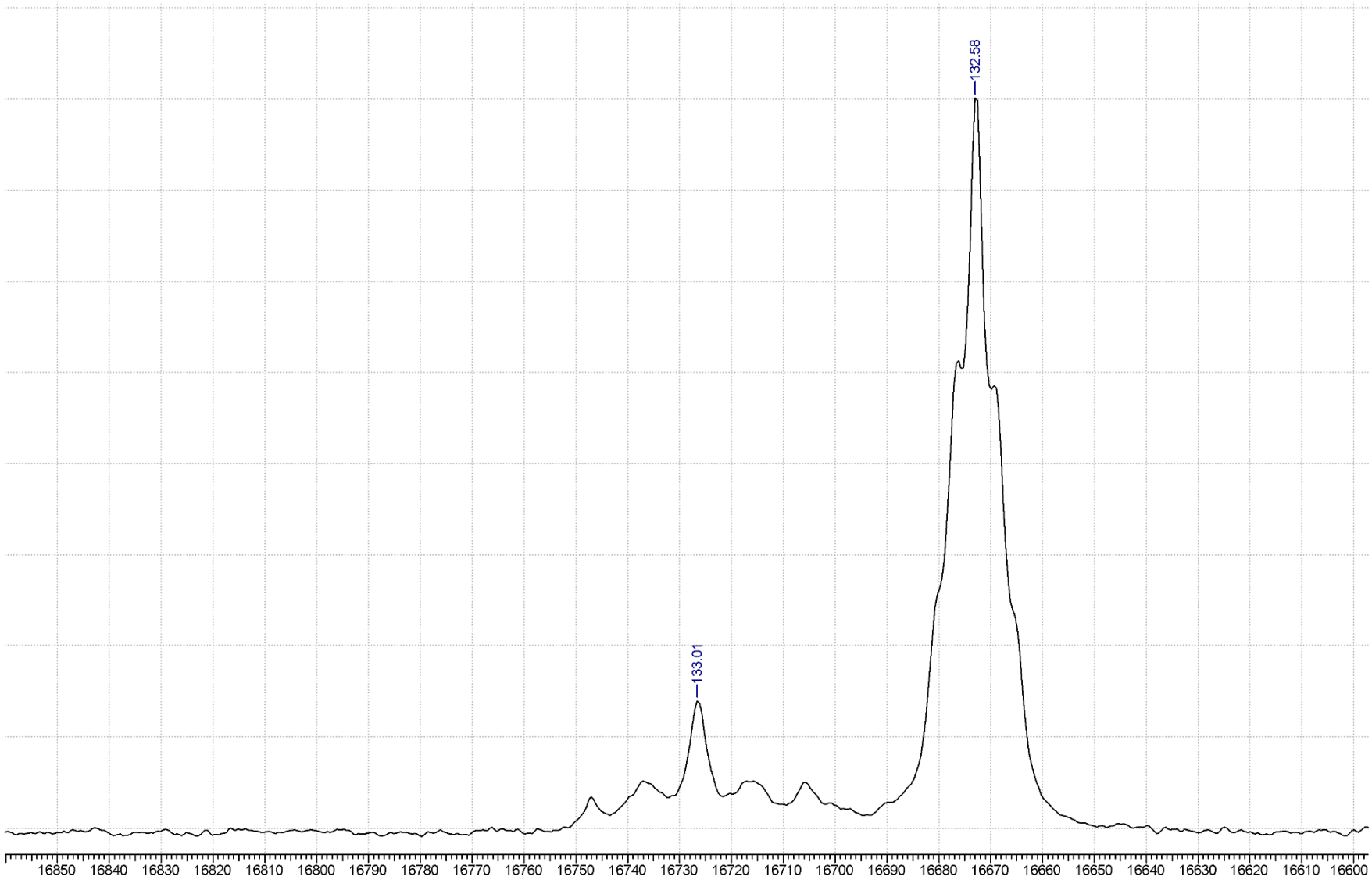


Figure S5. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, CD_2Cl_2, 298K, ppm) of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$ (16850–16600 Hz).



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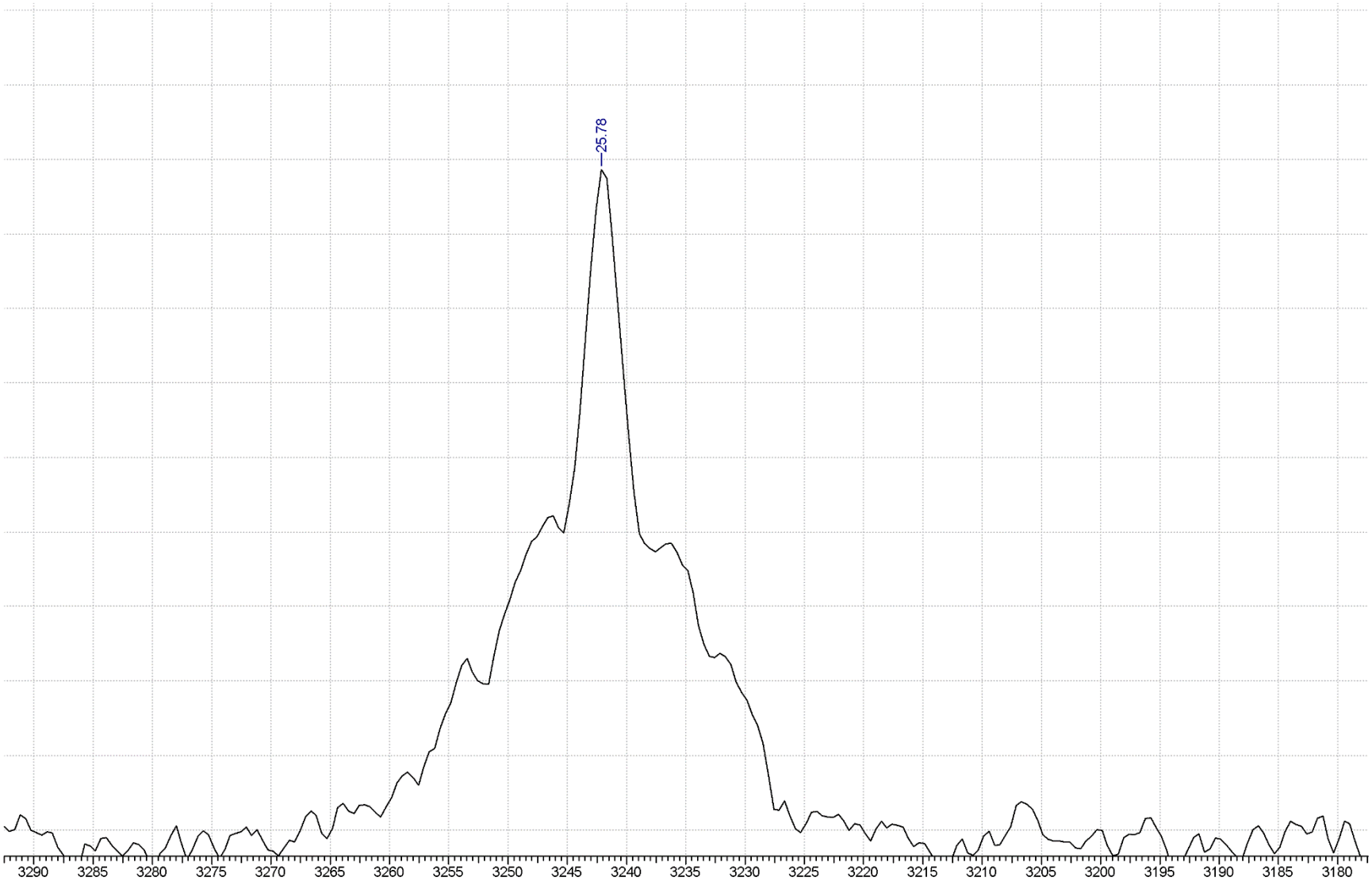


Figure S7. $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, CD_2Cl_2, 298K, ppm) in JMODECHO mode of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$.

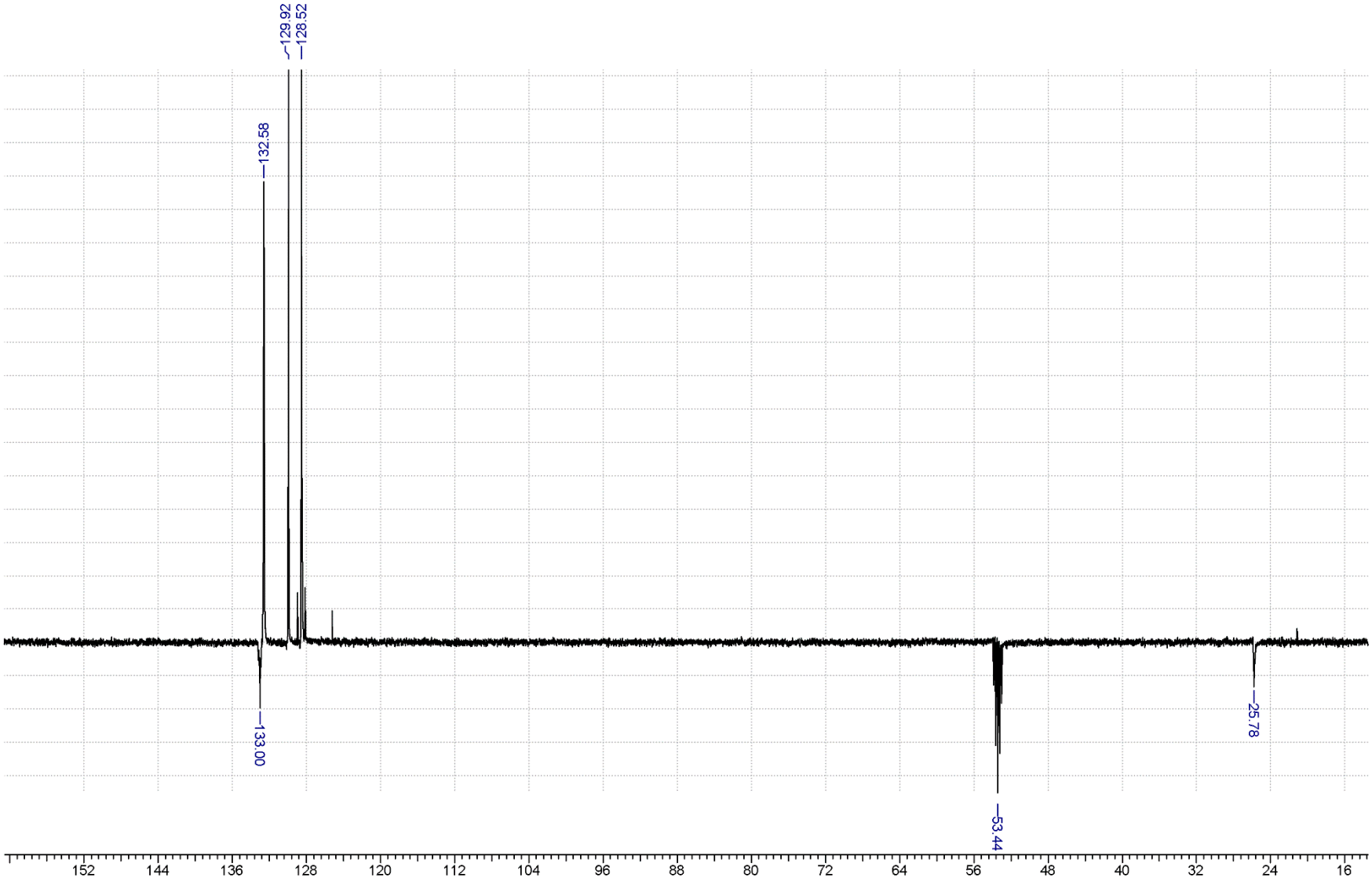


Figure S8. FTIR spectra of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$ in the KBr pellet.

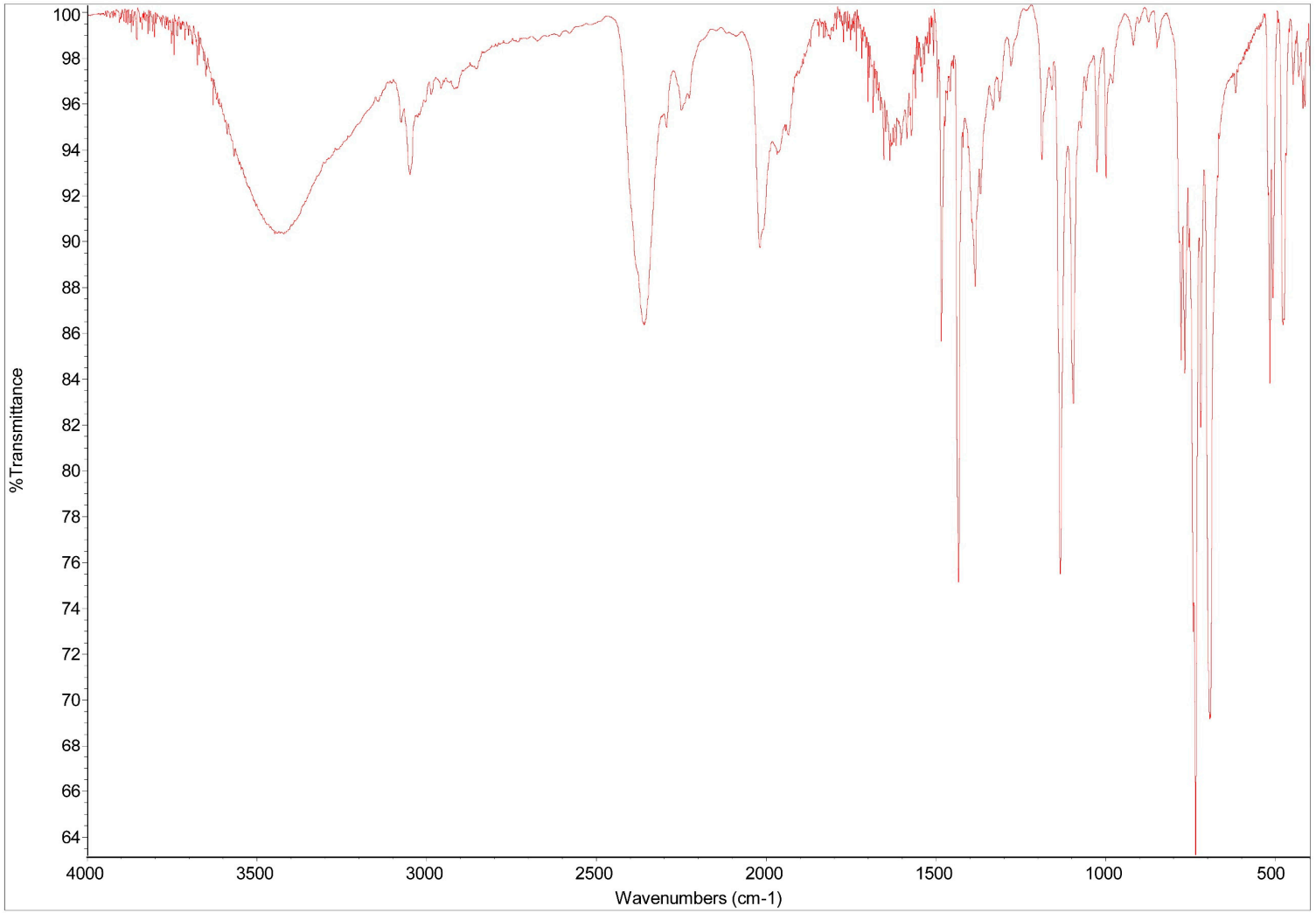


Figure S9. FTIR spectra of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$ in Nujol mull/thin polyethylene film.

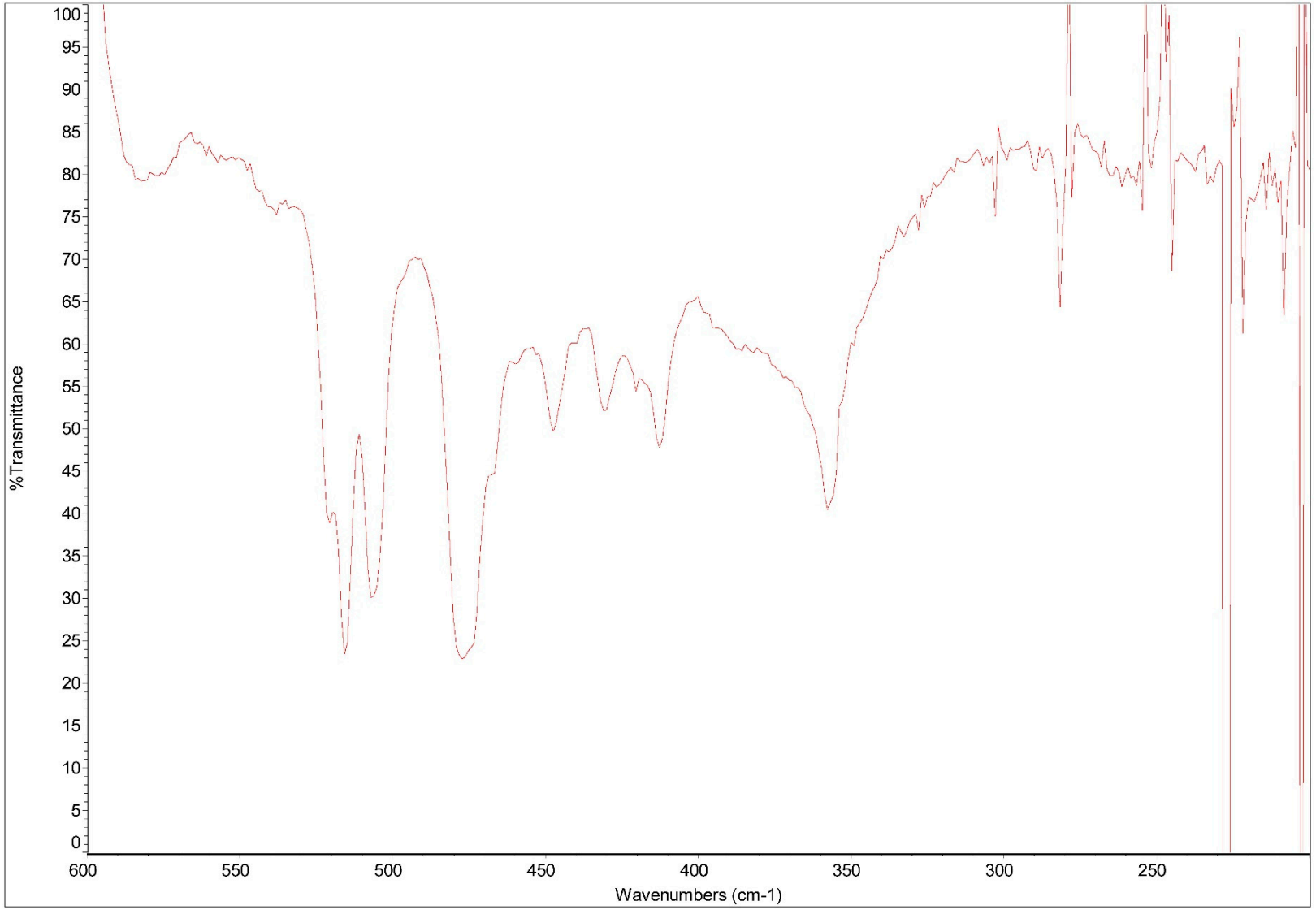
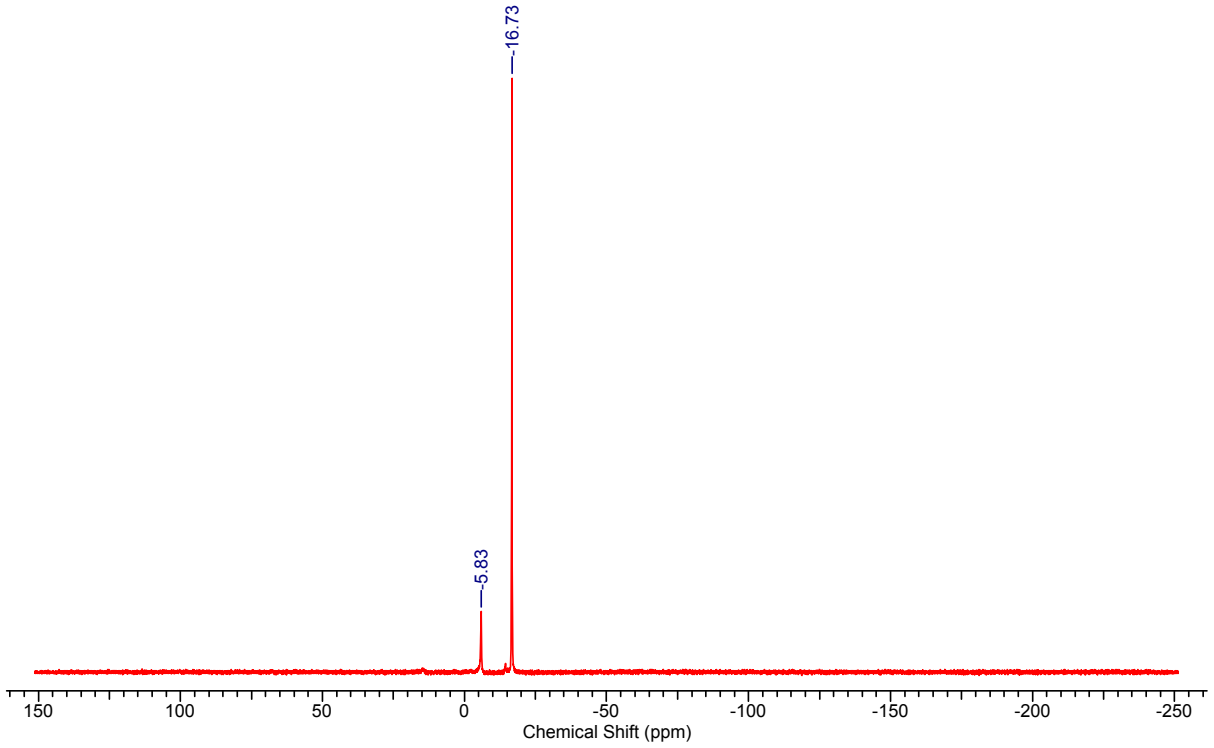
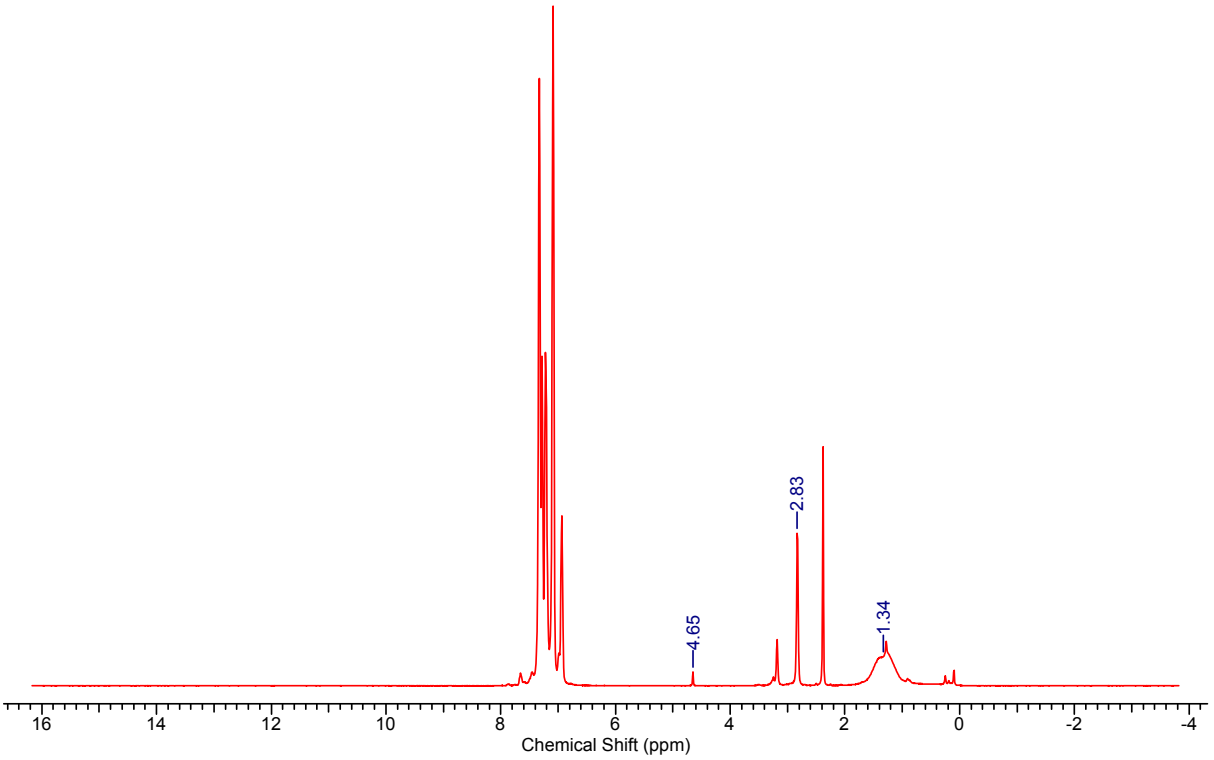


Figure S10. $^{31}P\{^{1}H\}$ (202 MHz, 298K, ppm) and ^{1}H NMR spectra (500 MHz, 298K, ppm) of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$ in $CDCl_3$.

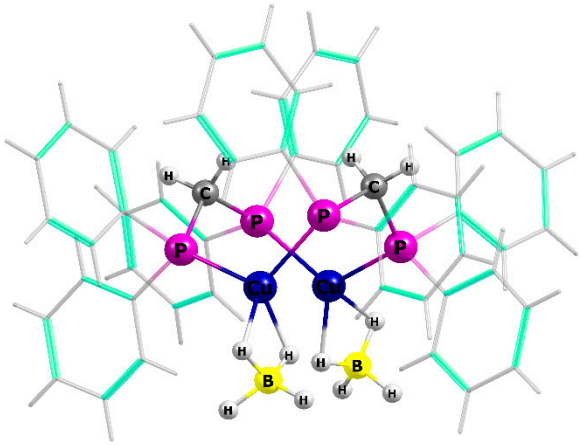


^{31}P NMR spectra of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$ in $CDCl_3$

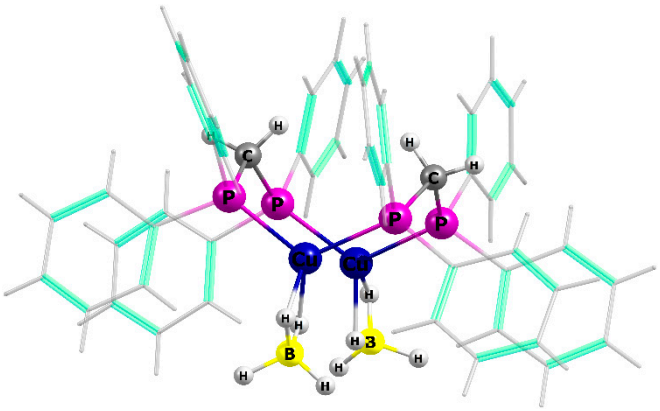


^{1}H NMR spectra of $[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$ in $CDCl_3$

Figure S11. General view of molecular structures of 1 and 2 conformations. The solvents molecules are omitted for clarity.



1 $[(\mu_2\text{-dppm})_2Cu_2(\eta^2\text{-}BH_4)_2]\cdot CH_2Cl_2$ orthorombic **($P2_12_12_1$)** ϱ_{calc} = 1.353 g/cm^3



2 $[(\mu_2\text{-dppm})_2Cu_2(\eta^2\text{-}BH_4)_2]\cdot 0.5CH_2Cl_2$ monoclinic **($P2_1/c$)** ϱ_{calc} = 1.328 g/cm^3

Table S1. CCDC analysis of the structures, containing eight-membered $[(\mu^2\text{-dppm})_2Cu_2]^{2+}$ moieties.

№	CSD refcode	Formula	Conf	δ^{31}P	Ligand	$l_{(Cu–Cu)}$	∠PCuP	Dih. angle	∠PCP	Ref
1.	SETDAW	$[(\mu_2\text{-dppm})_2Cu_2(\mu_2\text{-mpyO})]_2\cdot BF_4$	Boat-Boat	−9.2 (CDCl3)	mpyO	2.679	123/125	123-127	110/110	[1]
2.	NOFHIZ	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}C_6H_4(CO_2)_2)$ $Cu_2(\mu_2\text{-dppm})_2](PF_6)_2\cdot 3.4CH_2Cl_2$	Boat-Boat	–	$C_6H_4(CO_2)_2$	2.708	130/130	135/-127	112/112	[2]
3.	ELIKOZ	$[(\mu_2\text{-dppm})_2Cu_2(\mu_2\text{-}S_2NEt_2)][ClO_4]\cdot EtOH\cdot H_2O$	Distor. Boat-Chair	–	Et_2NS_2	2.712	133/134	119/-150	114/115	[3]
4.	AWUCIE	$[(\mu_2\text{-dppm})_2Cu_2(\mu_2\text{-SPh})(NCMe)][ClO_4]\cdot Et_2O$	Boat-Chair	–	PhS	2.735	125/128	129/-127	111/112	[4]
5.	ONUFEJ	$[(\mu_2\text{-dppm})_2Cu_2\{(S,S)\text{-}i\text{Pr-pybox}\}][PF_6]_2$ $\cdot 2CH_2Cl_2\cdot Et_2O$	Twisted Boat-Boat	–3.6 (d^6-Me2CO)	(S,S)-*i*Pr-pybox	2.743	124/140	164/-103	111/111	[5]
6.	JIQVUB	$(\mu_2\text{-dppm})_2Cu_2(2\text{-sba})\cdot 3CH_2Cl_2$	Distor. Boat-Chair	–9.8 (CDCl3)	2-sba	2.749	127/146	121/-154	110/110	[6]
7.	BUVPAK	$[(\mu_2\text{-dppm})_2Cu_2(N\text{^}N\text{^}O)][BF_4]_2$	Boat-Boat	–	N^N^O	2.781	119/120	119/-121	111/111	[7]
8.	NOQXAS	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}O_2CMe)][BF_4]\cdot Me_2CO$	Boat-Boat	–10.2 (CD3CN)	$MeCO_2$	2.789	129/131	124/-136	112/112	[8]
9.	NOFJUN	$[(\mu\text{-dppm})_2Cu_2$- $(O_2CC_2F_4CO_2)Cu_2(\mu\text{-dppm})_2](PF_6)_2\cdot 5CH_2Cl_2$	Boat-Boat	–	$C_2F_4(CO_2)_2$	2.833	125/134	136/-124	112/113	[2]
10.	CIYMIH	$[(\mu_2\text{-dppm})_2Cu_2][PF_6]_2\cdot 2CH_2Cl_2\cdot H_2O$	Distor. Boat-Chair	–7.0 (CD2Cl2)	–	2.833	132/134	144/-122	112/113	[9]
11.	IMOWOX	$[(\mu_2\text{-dppm})_2Cu_2(4\text{-}PyCO_2)]_4[BF_4]_4\cdot CH_2Cl_2$	Distor. Boat-Chair Boat-Boat	–7.9 (CDCl3)	$[4\text{-}PyCO_2]^-$	2.833 2.968	136/142 120/130	164/-127 125/-129	112/113	[10]
12.	CIYMUT	$1.5\ [(\mu_2\text{-dppm})_2Cu_2][PF_6]_2\cdot 2CH_2Cl_2$	Boat-Chair	–7.0 (CD2Cl2)	–	2.844 2.878 2.924	121/126 117/120 125/131	130/-124 116/-121 125/-131	112/114 112/113 111/115	[9]
13.	TADZOP	$[(\mu_2\text{-dppm})_2Cu_2(cca)(NO_3)(CH_3OH)]$	Boat-Boat	–	cca	2.847	124/126	123/-128	111/112	[11]
14.	TEQGED	$[(\mu_2\text{-dppm})_2Cu_2(N\text{^}N)_2][BF_4]_2$	Distor. Boat-Chair	−7.0 (CDCl3)	N^N	2.849	138/139	133/-160	114/115	[12]
15.	ETIQEF	$[\{(\mu_2\text{-dppm})_2Cu_2(\mu\text{-CN})\}_2][PF_6]_2$	Distor. Boat-Chair	−8.5/−10.5 (CD2Cl2)	CN	2.867	126/135	116/-150	112/113	[13]
16.	IMOWUD	$[(\mu_2\text{-dppm})_2Cu_2(6\text{-Me-}3\text{-}PyCO_2)]_4[BF_4]$	Boat-Boat	−7.8 (CDCl3)	6-Me-3-$PyCO_2$	2.869	129/130	133/-129	114/114	[10]
17.	CIYMON	$2\ [(\mu_2\text{-dppm})_2Cu_2][PF_6]_4\cdot CH_2Cl_2$	Boat-Chair	–7.0 (CD2Cl2)	–	2.874 2.950	123/124 126/130	123/-124 131/-119	111/113 114/115	[9]
18.	IPAHIQ	$[(\mu_2\text{-dppm})_2Cu_2(C_7H_7N)(\mu\text{-}NO_3)][NO_3]$	Boat-Boat	–10.9 (CDCl3) /–23.0 free dppm	NO_3^-	2.916	128/136	136/-133	110/111	[14]
19.	CAWKIV	$[(\mu_2\text{-dppm})_2Cu\{(CO_2)_2C_6H_2(Boc)_2\}]_2\cdot 11THF$	Twisted Boat-Chair	−8.2 (CDCl3)	$[(Boc)_2C_6H_2(CO_2)_2]^-$	2.925	122/130	105/-148	110/115	[15]
20.	XUJCIQ	$[(\mu_2\text{-dppm})_2Cu_2(OOCL)]_2[NO_3]_2$	Distor. Boat-Boat	–	–	2.931	119/120	134/-108	110/112	[16]
21.	SOMJAF	$[(\mu_2\text{-dppm})_2Cu_2][OC_6Cl_4OH]_2$	Boat-Chair	−6.3 (d^6-DMSO) /−18.6 dppm	$HOC_6Cl_4O^-$	2.944	130/131	137/-124	113/113	[17]
22.	SULYAZ	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}O_2CPh)][O_2CPh]\cdot H_2O$	Distor. Boat-Boat	–	$PhCO_2$	2.944	117/119	127/-111	110/112	[18]
23.	YIVSUT	$[(\mu_2\text{-dppm})_2Cu_2(tsmc)\}[NO_3]_2\cdot MeOH\cdot H_2O$	Boat-Chair	–	tsmc	2.956	126/130	128/-128	113/114	[19]
24.	LERFOE	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-HCOO})(C_7H_7N)][NO_3]$	Boat-Boat	−10.1 (CDCl3)	$HCOO^-/C_7H_7N$	2.958	125/132	132/-129	111/112	[20]
25.	TEDHUG	$[(\mu_2\text{-dppm})_2Cu_2][2\text{-pyO}]_2$	Boat-Boat	−11.2 (d^6-DMSO)	2-pyO^-	2.962	123/128	128/-128	110/112	[21]
26.	SIWYED	$[(\mu_2\text{-dppm})_2Cu_2][BOC\text{-}5,6\text{-anh-nc}]_2$	Twisted Boat-Boat	–	BOC-5,6-anh-nc	2.981	117/126	139/-103	109/113	[22]

27.	INOSOT	$[(\mu_2\text{-dppm})Cu][ttfac)]_2\cdot(C_4H_8O)_2$	–	−13.6 $_{(CDCl3)}$/ −23.0 free dppm	ttfac	2.986	–	–	–	[23]
28.	XUDKUD	$[(\mu_2\text{-dppm})_2Cu_2][tsac]_2\cdot CH_2Cl_2$	Twisted Boat-Boat	+46.35 $_{(d^6\text{-DMSO})}$	tsac	3.036	110/115	89/-138	109/112	[24]
29.	LEFBUW	$[(\mu_2\text{-dppm})_2Cu_2(fptz)][ClO_4]\cdot 2H_2O$	Distor. Boat-Boat	−11.4 $_{(CD2Cl2)}$	fptz	3.049	121/130	131/-120	114/114	[25]
30.	LEFBEG	$[(\mu_2\text{-dppm})_2Cu_2(m\text{-fmptz})][ClO_4]\cdot 2CH_2Cl_2$	Boat-Chair	−11.1 $_{(CD2Cl2)}$	m-fmptz	3.085	130/132	135/-127	114/115	[25]
31.	LEFBOQ	$[(\mu_2\text{-dppm})_2Cu_2(o\text{-bmptzH})][ClO_4]_2\cdot H_2O$	Distor. Boat-Boat	–	bmptzH	3.085	130/121	131/-120	114/114	[25]
32.	AZINEC	$[(\mu_2\text{-dppm})_2Cu_2(CN\textit{t}Bu)][BF_4]_2$	Boat-Boat	−2.13 $_{(CD2Cl2)}$	CN*t*Bu	3.100	118/122	125/-114	110/111	[26]
33.	LEFBIK	$[(\mu_2\text{-dppm})_2Cu_2(p\text{-fmptz})][ClO_4]\cdot 2H_2O$	Distor. Boat-Boat	−12.8 $_{(CD2Cl2)}$	p-fmptz	3.110	114/131	123/-121	113/114	[25]
34.	CAWKOB	$[(\mu_2\text{-dppm})_2Cu_2\{(CO_2)_2C_{10}H_4(Boc)_2\}]_2\cdot 3DME$	Twisted Boat-Boat	–	$(Boc)_2C_{10}H_4(CO_2)_2$	3.119	124/126	94/-156	109/110	[15]
35.	IMOWIR	$[(\mu_2\text{-dppm})_2Cu_2(3\text{-}PyCO_2)]_2(BF_4)_2\cdot 4CH_2Cl_2$	Distor. Boat-Boat	−8.0 $_{(CDCl3)}$	3-$PyCO_2$	3.126	122/123	115/-132	112/113	[10]
36.	IMOWEN	$[(\mu_2\text{-dppm})_2Cu_2(2\text{-}PyCO_2)]_2(BF_4)_2$	Twisted Boat-Chair	−7.7 $_{(CDCl3)}$	2-$PyCO_2$	3.133	120/132	108/-145	112/115	[10]
37.	VOFWOD	$[\{(o\text{Tol})_2PCH_2P(o\text{Tol})_2\}CuCl]_2\cdot 2C_2H_4Cl_2$	Twisted Boat-Boat	−18.4 $_{(CDCl3)}$	Cl^-	3.133	119/119	90/-149	109/110	[27]
38.	LEFBAC	$[(\mu_2\text{-dppm})_2Cu_2(o\text{-fmptz})][ClO_4]\cdot 2CH_2Cl_2$	Boat-Chair	−10.9/$_{(CD2Cl2)}$ −9.6	o-fmptz	3.136	129/133	128/-134	115/115	[25]
39.	HOSXOC	$[(\mu_2\text{-dppm})_2Cu_2(Me_2NCN)_3][BF_4]_2$	Boat-Boat	−10.0 $_{(CDCl3)}$	Me_2NCN	3.143	115/125	118/-123	110/113	[28]
40.	TOMKOW	$[(\mu_2\text{-dppm})_2Cu_2\{(\mu_3\text{-}S)_2Mo_2(\mu\text{-}S)_2(edt)_2\}(Py)]\cdot Py$	Boat-Boat	–	$(\mu_3\text{-}S)_2Mo_2(\mu\text{-}S)_2(edt)_2$	3.159	113/113	113/-113	112/113	[29]
41.	YUMKEY	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}Cl)(i\text{-}C_9H_7N)_2][Cl]$	Boat-Boat	−15.2 $_{(CDCl3)}$	Cl^-/*i*-C_9H_7N	3.163	121/124	121/-125	114/114	[30]
42.	GIPNOJ	$\{[\{(\mu_2\text{-dppm})_2Cu_2\}_2(\mu\text{-eddbn})]\ [PF_6]_4\cdot 11CH_2Cl_2\}_n$	Boat-Boat	−8.0 $_{(CD2Cl2)}$ /−21.1	eddbn	3.166	123/125	125/-123	111/112	[31]
43.	SACKUE	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-NCMe})(NCMe)_2][ClO_4]_2$	Boat-Chair	–	MeCN	3.168	130/132	131/-131	112/114	[32]
44.	NIKBAK	$[(\mu_2\text{-dppm})_2Cu_2][NO_3]_2$	Distor. Boat-Boat	–12.3 $_{(CDCl3)}$	NO_3^-	3.170	132/132	122/-142	112/112	[33]
45.	**2**/[dppmCuBH$_4$]$_2$	$[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$	Boat-Boat	−14.6 $_{(CD2Cl2)}$	BH_4^-	3.204	117/118	117/-118	111/111	this work
46.	GIPPIF	$[\{(\mu_2\text{-dppm})_2Cu_2\}_2(\mu\text{-bpdcn})]\ [BF_4]_2\cdot CH_2Cl_2$	Distor. Boat-Chair	–	bpdcn	3.213	124/138	142/-121	113/114	[31]
47.	GIPPAX	$\{[\{(\mu_2\text{-dppm})_2Cu_2\}_2(\mu_2\text{-}1,4\text{-bcpvb})(\mu\text{-}1,4\text{-bcpvb})][PF_6]_4\cdot 10CH_2Cl_2\}_n$	Boat-Boat	–	1,4-bcpvb	3.223	121/127	124/-124	111/112	[31]
48.	GIPNUP	$\{[\{(\mu_2\text{-dppm})_2Cu_2\}_2(\mu_2\text{-bpdcn})(\mu\text{-bpdcn})][PF_6]_4\cdot 13CH_2Cl_2\}_n$	Boat-Boat	–	bpdcn	3.235	133/134	131/-136	111/112	[31]
49.	GIPPEB	$\{[\{(\mu_2\text{-dppm})_2Cu_2\}_2(\mu_2\text{-tddeddbn})(\mu\text{- tddeddbn})][PF_6]_4\cdot 8CH_2Cl_2\}_n$	Boat-Boat Twisted-Boat	–	tddeddbn	3.243 3.224	123/127 115/115	126/-124 93/-138	110/114 110/110	[31]
50.	BUPYOB	$[(\mu_2\text{-dppm})_2Cu_2\{SP(O\textit{i}Pr)_2NC(S)NHPh)\}I\cdot Me_2CO$	Distor. Boat-Boat	–25.7 ÷ –12.2 $_{(d^6\text{-DMSO})}$	$SP(O\textit{i}Pr)_2NC(S)NHPh$	3.246	109/110	117/-102	113/113	[34]
51.	FIWWEO	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}SCN)_2]\cdot 3MeCN$	Boat-Boat	–	SCN^-	3.248 3.257	113/117 113/115	116/-115 111/-117	113/115	[35]
52.	YUMKOI	$[(\mu_2\text{-dppm})_2Cu_2(4,4\text{-biPy})(\mu\text{-}Cl)][Cl]\cdot 4MeCN$	Boat-Boat	–	Cl^-/4,4-biPy	3.264	116/122	120/-118	112/114	[30]
53.	OLARUQ	$[\{(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}2,2\text{-biPy-tzl})\}_2][ClO_4]_2\cdot 2Me_2CO$	Distor. Boat-Chair	–18.0/ –12.4 $_{(CD2Cl2)}$	2,2-biPy-tzl	3.288	117/143	118/-145	115/118	[36]
54.	HOMVEK	$[(\mu_2\text{-dppm})_2Cu_2(Me_2NCN)(\mu\text{-}Cl)][Cl]\cdot 2Me_2NCN$	Distor. Boat-Boat	–15.2 $_{(CDCl3)}$	Cl^-/Me_2NCN	3.293	125/125	121/-130	114/115	[37]

55.	BUVPEO	$[(\mu_2\text{-dppm})_2Cu_2(N\text{^}C\text{^}N)][BF_4]_2\cdot 3CH_2Cl_2$	Boat-Boat	−11.2 (DMSO)	N^C^N	3.294 3.314	132/132 129/129	129/-135 130/-129	114/114 115/115	[7]
56.	BEBPOO	$[(\mu_2\text{-dppm})_2Cu_2(\text{Py-2,6-}CO_2)][NO_3]_2$	Distor. Boat-Chair	−13.9 ($CDCl_3$)	Py-2,6-CO_2	3.298	125/131	114/-143 143/-114	114/114	[38]
57.	ZEBLAW	$[(\mu_2\text{-dppm})_2Cu_2(\mu_2\text{-MeCN})(MeCN)_2][BF_4]_2\cdot CH_2Cl_2$	Distor. Boat-Boat	–	MeCN	3.313 3.389	122/131 119/133	128/-126 132/-122	112/115 112/114	[39]
58.	YUMLAV	$\{[(\mu_2\text{-dppm})_2Cu_2(4,4\text{-biPy})(\mu\text{-Cl})][ClO_4]\}_n$	Boat-Boat	–	Cl^-/4,4-biPy	3.328	122/122	120/-124	114/114	[30]
59.	SULXUS	$[(\mu_2\text{-dppm})_2Cu_2(O_2CPh)_2]$	Chair-Chair	–	$PhCO_2$	3.359	144/144	180/180	112/112	[18]
60.	SOFQUA	$[(\mu_2\text{-dppm})_2Cu_2(C_9H_7N)(\mu\text{-Cl})][Cl]\cdot C_9H_7N\cdot C_{10}H_8\cdot MeCN$	Distor. Boat-Boat	–	Cl^-/C_9H_7N	3.364	111/120	113/-120	114/114	[40]
61.	NEPSOS	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}C_3H_8N_2S)][I]_2\cdot 1.5MeCN$	Distor. Boat-Boat	–	$I^-/C_3H_8N_2S$	3.375	117/120	113/-124	114/117	[41]
62.	PUSMEX	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}C_4H_8N_2S)][Br]_2\cdot 2MeCN$	Distor. Boat-Boat	–	$Br^-/C_4H_8N_2S$	3.378	116/119	123/-113	113/117	[42]
63.	IXOMOY	$[(\mu_2\text{-dppm})_2Cu_2\{\mu\text{-3,6-(2-Py)2-4,5-(4-Py)Pydz}\}][NO_3]_2\cdot H_2O$	Boat-Chair	−6.5 ($CDCl_3$)	3,6-(2-Py)2-4,5-(4-Py)Pydz	3.390	124/131	129/-127	114/115	[43]
64.	IXONAL	$[(\mu_2\text{-dppm})_2Cu_2\{\mu\text{-3,6-(2-Py)2-4,5-(4-Py)Pydz}\}][NO_3]_2\cdot CH_2Cl_2$	Boat-Chair	−6.5 ($CDCl_3$)	3,6-(2-Py)2-4,5-(4-Py)Pydz	3.390	124/131	127/-129	114/116	[43]
65.	SIBDUD	$\{[(\mu_2\text{-dppm})_2Cu_2\{Mo(mnt)_3\}(MeCN)]\cdot MeCN\cdot 2Et_2O\}_n$	Boat-Boat	–	$[Mo(mnt)_3]^{2-}$/MeCN	3.391	116/125	121/-121	114/116	[44]
66.	**1**/$[dppmCuBH_4]_2$	$[(\mu_2\text{-dppm})_2Cu_2][\eta^2\text{-}BH_4]_2$	Twisted Boat-Boat	−14.6 (CD_2Cl_2)	BH_4^-	3.392	111/113	134/-92	111/113	this work
67.	REWBIF	$\{[(\mu_2\text{-dppm})_2Cu_2\{W(mnt)_3\}(MeCN)]\cdot MeCN\cdot 2Et_2O\}_n$	Boat-Boat	–	$[W(mnt)_3]^{2-}$/MeCN	3.395	116/125	121/-121	114/116	[45]
68.	IXOMUE	$[(\mu_2\text{-dppm})_2Cu_2\{\mu\text{-3,6-(2-Py)2-4,5-(Ph)Pydz}\}][NO_3]_2\cdot CH_2Cl_2$	Boat-Boat	−8.1($CDCl_3$)	3,6-(2-Py)2-4,5-(Ph)Pydz	3.406	125/130	129/-126	114/117	[43]
69.	QITFUW	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-pmk})][BF_4]_2$	Distor. Boat-Boat	−11.2 ($CDCl_3$)	pmk	3.417	114/114	106/-123	114/114	[46]
70.	BUVPOY	$[(\mu_2\text{-dppm})_2Cu_2(paa)][BF_4]_2$	Boat-Boat	–	paa	3.420	114/114	112/-118	113/113	[7]
71.	HOSXUI	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}ClO_4)(Me_2CN)_2][ClO_4]$	Boat-Chair	−10.9 ($CDCl_3$)	ClO_4^-/ Me_2CN	3.424	131/133	131/-135	112/115	[28]
72.	DEDFEX	$[(\mu_2\text{-dppm})_2Cu_2][\mu\text{-}S_2C(o\text{Tol})]_2$	Distor. Boat-Boat	–	$[S_2C(o\text{Tol})]^-$	3.426	114/114	101/-129	111/111	[47]
73.	KIKBEL	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-PPDMe})][BF_4]_2$	Boat-Chair	−7.4 (CD_2Cl_2)	PPDMe	3.452	125/130	124/-132	115/116	[48]
74.	AFOJEL	$\{[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-Cl})((\mu_2\text{-TCNQ})\}_n$	Distor. Boat-Boat	−13.4 (d^7-DMF)	Cl^-/TCNQ	3.454	95/130	107/-87	113/115	[49]
75.	SOFQIO	$[(\mu_2\text{-dppm})_2Cu_2(C_9H_7N)(\mu\text{-Cl})][Cl]\cdot 2C_9H_7N\cdot H_2O$	Distor. Boat-Boat	–	Cl^-/Me_2NCN	3.467	111/118	122/-108	114/114	[40]
76.	CAHKAZ	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}L_{NN})][BF_4]_2\cdot 4H_2O$	Boat-Boat	–	L_{NN}	3.637	124/128	127/-130	114/115	[50]
77.	NOVHUB	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}NO_3)(Py)_2][NO_3]_2\cdot CH_3OH$	Boat-Boat	−10.8 ($CDCl_3$)	NO_3/Py	3.651	126/126	128/-128	112/113	[51]
78.	PUXJAT	$[(\mu_2\text{-dppm})_2Cu_2][ttfa]_2$	Twisted Boat-Boat	–	ttfa	3.663	115/115	144/-92	113/113	[52]
79.	NIWKAG	$\{[(\mu_2\text{-dppm})_2Cu_2(4,4\text{-biPy})][BF_4]_2\cdot 2.5CH_2Cl_2\}_n$	Distor. Boat-Boat	–	4,4-biPy	3.713	122/130	115/-142	111/117	[53]
80.	QIFZIO	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-TePh})][BF_4]$	Boat-Chair	−6.9 (d^6-acetone)	TePh	3.723	128/129	129/-131	112/114	[54]
81.	CECNAA	$[(\mu_2\text{-dppm})_2Cu_2\{S_2P(O\textit{i}Pr)_2\}]\cdot 2CH_2Cl_2$	Twisted Boat-Boat	+2.1 ($CDCl_3$)	$S_2P(O\textit{i}Pr)_2$	3.736	111/111	93/-134	115/115	[55]
82.	QIFZEK	$[(\mu_2\text{-dppm})_2Cu_2(\mu\text{-SePh})(Me_2CO)][BF_4]\cdot Et_2O$	Boat-Chair	−6.3 (d^6-acetone)	SePh/Me_2CO	3.739	128/129	130/-129	112/113	[54]
83.	WEGSOR	$[(\mu_2\text{-dppm})_2Cu_2(4\text{-vinylPy})_2(\mu\text{-HCOO})][PF_6]$	Distor. Boat-Boat	−10.6 ($CDCl_3$)	HCOO/4-vinylPy	3.742	119/127	129/-122	115/115	[56]

84.	QITGAD	$[(\mu_2\text{-dppm})_2Cu_2(MeCN)_4][BF_4]_2$	Distor. Boat-Boat	−7.9 (CDCl3)	MeCN	3.755	120/120	108/-137	114/114	[46]
85.	OLASAX	$[\{(\mu_2\text{-dppm})_2Cu_2(\mu\text{-}4,4\text{-Me-}2,2\text{-biPy-tzl})\}_2][ClO_4]_2\cdot 2Me_2CO$	Distor. Boat-Chair	−18.7/(CD2Cl2) −12.6	4,4-Me-2,2-biPy-tzl	3.756 3.907	115/139 121/137	113/-146 151/-115	118/121 121/122	[36]
86.	WABHEN	$[(\mu_2\text{-dppm})_2Cu_2(MeCN)_4][PF_6]_2$	Twisted Boat-Boat	–	MeCN	3.756	120/120	138/-107	114/114	[57]
87.	FEWVAE	$[(\mu_2\text{-dppm})_2Cu_2(MeCN)_4][ClO_4]_2$	Twisted Boat-Boat	–	MeCN	3.757	120/120	138/-107	113/113	[58]
88.	CODSUK	$[(\mu_2\text{-dppm})_2Cu_2(pht)_2]\cdot THF$	Chair-Chair	–	pht	3.776	132/132	180/-180	110/110	[59]
89.	CATHAH	$[(\mu_2\text{-dppm})_2Cu_2(Bzm)_2(\mu\text{-}NO_3)][NO_3]$	Distor. Boat-Boat	–	Bm	3.852	127/127	139/-122	116/116	[60]
90.	SUHFIK	$[(\mu_2\text{-dppm})_2Cu_2(\{\mu\text{-}4\text{-}(4\text{-Cl-styryl})Py\}_2(\mu\text{-}ClO_4)][ClO_4]$	Distor. Boat-Chair	–	4-(4-Cl-styryl)Py/ClO4−	3.865	132/137	153/-125	115/117	[61]
91.	QUHMAI	$\{[(\mu_2\text{-dppm})_2Cu_2(4,4\text{-biPy})(\mu\text{-}CF_3SO_3)][CF_3SO_3]\cdot MeOH\}_n$	Boat-Chair	−12.2 (d^6-DMSO)	4,4-biPy/CF_3SO_3	3.901	128/137	137/-138	115/116	[62]
92.	OXIFAD	$\{[(\mu_2\text{-dppm})_2Cu_2(4\text{-}CF_3pymS)_2]\cdot 2MeCN$	Chair-Chair	23.0 (CDCl3)	4-CF_3pymS	3.904	130/130	180/-180	114/114	[63]
93.	KANQOG	$[(\mu_2\text{-dppm})_2Cu_2(Py\text{-}2\text{-}CO_2)_2][NO_3]_2$	Chair-Chair	−14.4 (CDCl3)	Py-2-CO_2	4.068	140/140	180/-180	112/112	[64]
94.	GOMDES	$\{[(\mu_2\text{-dppm})_2Cu_2(\mu_2\text{-pyz})][ClO_4]_2\cdot CH_2Cl_2\}_n$	Chair-Chair	–	pyz	4.116	145/145	180/-180	115/115	[65]
95.	QUHLUB	$[(\mu_2\text{-dppm})_2Cu_2(\mu_2\text{-pyz})][(BF_4]_2\cdot(CH_2Cl_2)_2\}_n$	Chair-Chair	−12.1 (d^6-DMSO)	pyz	4.120	145/145	180/-180	116/116	[62]
96.	EREHUF	$[(\mu_2\text{-dppm})_2Cu_2\{\mu\text{-}3,5\text{-}(6\text{-}2,2\text{-biPy})Pzl\}][NO_3]_2$	Plain(boat)	–	3,5-(6-2,2-biPy)Pzl	4.277	148/150	170/-170	117/117	[66]
97.	FERLIZ	$[(\mu_2\text{-dppm})_2Cu_2(BrbiPyBr)_2][ClO_4]_2\cdot 2CH_2Cl_2$	Chair-Chair	–	BrbiPyBr	4.433	135/135	180/180	116/116	[67]
98.	RIRRIV	$[(\mu_2\text{-dppm})_2Cu_2(Bphen)_2][BF_4]_2\cdot CH_2Cl_2$	Distor. Boat-Chair	−6.6 (CD2Cl2)	Bphen	4.464	135/141	171/-154	116/116	[68]
99.	EVOXUK02	$[\{(\mu_2\text{-dppm})_2Cu(Hbmp)\}_2][ClO_4]_2\cdot 2CH_2Cl_2$	Chair-Chair	–	Hbmp	4.585	135/135	180/-180	120/120	[69]
100	YEHXAL	$[(\mu_2\text{-dppm})_2Cu_2(5\text{-}NO_2\text{-}1,10\text{-Phen})_2][ClO_4]_2$	Chair-Chair	–	5-NO_2-1,10-Phen	4.595	136/136	180/180	116/116	[70]
101	UJOQEP	$[(\mu_2\text{-dppm})_2Cu_2(1,10\text{-Phen})_2][NO_3]_2\cdot 6H_2O$	Chair-Chair	–	1,10-Phen	4.598	136/136	180/-180	117/117	[71]
102	BUDGOX	$[(\mu_2\text{-dppm})_2Cu_2(2,2'\text{-biPy})_2][BF_4]_2$	Chair-Chair	–	2,2'-biPy	4.599	137/137	180/-180	117/117	[72]
103	YEHXEP	$[(\mu_2\text{-dppm})_2Cu_2(NMP)_2][ClO_4]_2$	Chair-Chair	–	NMP	4.633	135/135	180/180	116/116	[70]
104	VIMQUD01	$[(\mu_2\text{-dppm})_2Cu_2(2,2'\text{-biPy})_2][NO_3]_2$	Chair-Chair	−9.9 (CDCl3)	2,2'-biPy	4.637	134/134	180/-180	147/147	[73]
105	YUMKUO	$[(\mu_2\text{-dppm})_2Cu_2(2,2'\text{-biPy})_2][CF_3SO_3]_2$	Distor. Boat-Chair	−15.2 (CDCl3)	2,2'-biPy	4.644	134/138	158/-171	117/119	[30]
106	UFADAH	$[(\mu_2\text{-dppm})_2Cu_2(2,2'\text{-biPy})_2][BF_4]_2\cdot 2Et_2O$	Chair-Chair	–	2,2'-biPy	4.671	133/133	180/180	117/117	[74]
107	MOFJIC	$[(\mu_2\text{-dppm})_2Cu_2(BrPhenBr)_2][Cl]_2\cdot 2CH_2Cl_2$	Chair-Chair	−10.0/(d^6-DMSO) −5.3	BrPhenBr	4.679	136/136	179/179	117/118	[75]
108	YUMKIC	$[(\mu_2\text{-dppm})_2Cu_2(1,10\text{-Phen})_2][Cl]_2\cdot 5H_2O$	Chair-Chair	−15.2 (CDCl3)	1,10-Phen	4.700	135/135	-180/-180	118/118	[30]
109	TICNIE	$[(\mu_2\text{-dppm})_2Cu_2(2\text{-Py-}CH_2\text{-}6\text{-Cou})_2][ClO_4]_2\cdot CH_2Cl_2$	Chair-Chair	–	2-Py-CH_2-6-Cou	4.709 4.775	133/133 134/134	180/-180 -180/-180	119/119 118/118	[76]
110	SAZFOP	$[(\mu_2\text{-dppm})_2Cu_2(1,10\text{-Phen})_2][BF_4]_2\cdot 2CH_2Cl_2$	Chair-Chair	–	1,10-Phen	4.720	133/133	180/180	119/119	[77]
111	JOGNUO	$[(\mu_2\text{-dppm})_2Cu_2(1,10\text{-Phen})_2][PF_6]_2\cdot 2Me2CO$	Chair-Chair	−5.6 (d^6-acetone)	1,10-Phen	4.742	134/134	180/-180	120/120	[78]
112	YESXOK	$[(\mu_2\text{-dppm})_2Cu_2\{SiMe_3C\equiv C\text{-}2,2'\text{biPy-}C\equiv C\ SiMe_3\}_2][ClO_4]_2$	Chair-Chair	−9.6 (CDCl3)	$SiMe_3C\equiv C$-2,2'biPy-$C\equiv C\ SiMe_3$	4.747 4.797	135/135 130/130	180/-180 180/-180	117/117 117/117	[79]

vdW radii Cu = 1.4 Å – ΣvdW(2Cu) = 2.8 Å

Table S2. Structural parameters of crystal structure **1** (Twisted Boat-Boat) and optimized structures.

Distances, Å	1	M06	PBE0	PBE0-D2	PBE0-D3BJ	B3LYP	B3LYP-D2	B3LYP-D3BJ	BP86	BP86-D2	BP86-D3BJ
Cu(1)···Cu(2)	3.392(1)	3.398	3.439	3.164	3.145	3.760	3.237	3.216	3.616	3.135	3.062
Cu(1)–P(2)	2.238(2)	2.277	2.268	2.234	2.243	2.304	2.258	2.268	2.262	2.219	2.228
Cu(2)–P(1)	2.253(2)	2.282	2.273	2.235	2.245	2.315	2.266	2.273	2.269	2.230	2.234
Cu(1)–P(3)	2.254(2)	2.282	2.271	2.233	2.246	2.315	2.263	2.271	2.270	2.230	2.334
Cu(2)–P(4)	2.257(2)	2.277	2.267	2.228	2.240	2.303	2.257	2.267	2.260	2.222	2.224
Cu(1)–B(1)	2.194(9)	2.196	2.195	2.176	2.185	2.239	2.206	2.216	2.202	2.170	2.184
Cu(2)–B(2)	2.190(7)	2.196	2.195	2.175	2.183	2.240	2.214	2.214	2.203	2.180	2.182
Cu(1)–H(1)BA	1.7682	1.776	1.774	1.754	1.756	1.810	1.772	1.767	1.781	1.747	1.746
Cu(1)–H(1)BB	1.8956	1.839	1.819	1.810	1.823	1.848	1.826	1.850	1.816	1.795	1.823
B(1)–H(1)BA	1.12	1.278	1.286	1.286	1.285	1.271	1.271	1.270	1.287	1.288	1.285
B(1)–H(1)BB	1.12	1.270	1.280	1.280	1.278	1.265	1.268	1.262	1.280	1.283	1.277
B(1)–H(1)BC	1.12	1.207	1.215	1.215	1.215	1.206	1.205	1.205	1.214	1.213	1.214
B(1)–H(1)BD	1.12	1.207	1.215	1.216	1.215	1.206	1.207	1.206	1.215	1.215	1.215
Cu(2)– H(2)BA	1.9398	1.839	1.824	1.806	1.820	1.852	1.851	1.845	1.823	1.815	1.817
Cu(2)– H(2)BB	1.6944	1.776	1.773	1.755	1.755	1.807	1.775	1.767	1.780	1.759	1.745
B(2)–H(2)BA	1.12	1.270	1.279	1.281	1.278	1.264	1.263	1.263	1.279	1.278	1.278
B(2)–H(2)BB	1.119	1.278	1.286	1.286	1.285	1.271	1.271	1.270	1.287	1.284	1.285
B(2)–H(2)BC	1.12	1.207	1.215	1.215	1.215	1.206	1.207	1.205	1.215	1.216	1.214
B(2)–H(2)BD	1.12	1.207	1.215	1.216	1.215	1.206	1.208	1.206	1.215	1.217	1.215
H(1)BB···H(2)BA	3.1143	2.909	3.090	2.722	2.713	3.722	2.673	2.836	3.422	2.464	2.574
B(1)···B(2)	5.06(1)	5.363	5.517	4.217	5.175	6.145	5.065	5.293	5.847	4.880	5.051
H(19)A···Cl(1')	2.722	–	–	–	–	–	–	–	–	–	–
H(13)A···Cl(1')	2.727	–	–	–	–	–	–	–	–	–	–
H(29)A···Cl(1')	2.816	–	–	–	–	–	–	–	–	–	–
H(28)A···Cl(1')	2.627	–	–	–	–	–	–	–	–	–	–
H(1)BD···Cl(2')	2.814	–	–	–	–	–	–	–	–	–	–
Angles,°	1	M06	PBE0	PBE0-D2	PBE-D3BJ	B3LYP	B3LYP-D2	B3LYP-D3BJ	BP86	BP86-D2	BP86-D3BJ

P(2)–Cu(1)–P(3)	112.93(7)	111.584	118.067	113.251	113.464	121.080	115.889	112.025	120.230	115.438	110.573
H(1)BA–Cu(1)–H(1)BB	60.95	70.604	71.273	71.987	71.539	68.728	70.149	69.530	71.004	72.470	71.591
P(1)–Cu(2)–P(4)	111.33(6)	111.590	118.351	113.463	113.214	120.968	115.393	111.673	121.232	114.441	110.150
H(2)BA–Cu(2)–H(2)BB	60.84	70.604	71.194	72.038	71.603	68.697	69.447	69.622	70.845	71.590	71.782
P(1)–C(1)–P(2)	112.6(3)	108.993	111.059	105.982	111.059	113.863	108.332	107.842	112.360	106.433	105.431
P(3)–C(2)–P(4)	109.9(4)	108.991	110.962	106.198	110.962	114.088	108.847	107.641	112.508	106.816	105.326
Cu(1)–H(1)BA–B(1)	96.3	90.455	90.206	90.084	90.206	91.543	91.411	92.240	90.270	89.964	90.922
Cu(1)–H(1)BB–B(1)	89.6	87.904	88.428	87.795	88.428	89.988	89.106	88.683	88.919	88.040	87.738
Cu(2)–H(2)BA–B(2)	87.1	87.901	88.242	87.906	88.242	89.854	88.497	88.765	88.688	87.844	87.850
Cu(2)–H(2)BB–B(2)	100.2	90.461	90.280	89.977	90.280	91.664	91.706	92.123	90.379	90.134	90.816
C(19)–H(19)A···Cl(1')	150.9	–	–	–	–	–	–	–	–	–	–
C(13)–H(13)A···Cl(1')	140.8	–	–	–	–	–	–	–	–	–	–
C(29)–H(29)A···Cl(1')	136.0	–	–	–	–	–	–	–	–	–	–
C(28)–H(28)A···Cl(1')	150.4	–	–	–	–	–	–	–	–	–	–
B(1)–H(1)BD···Cl(2')	142.6	–	–	–	–	–	–	–	–	–	–
Dihedral Angles,°	**1**	**M06**	**PBE0**	**PBE0-D2**	**PBE-D3BJ**	**B3LYP**	**B3LYP-D2**	**B3LYP-D3BJ**	**BP86**	**BP86-D2**	**BP86-D3BJ**
χ_1(P,Cu,Cu,P)	−92.41(6)	−87.634	−92.646	-83.909	−84.431	−99.810	-88.029	−83.833	−95.140	-86.784	-83.875
χ_2(P,Cu,Cu,P)	133.69(6)	137.091	146.124	144.279	143.359	147.675	144.838	141.351	148.106	144.253	137.410

Table S3. The differences between structural parameters of crystal structure **1** (Twisted Boat-Boat) and optimized structures.

Distances, Å	1	Δ[M06]	Δ[PBE0]	Δ[PBE0-D2]	Δ[PBE0-D3BJ]	Δ[B3LYP]	Δ[B3LYP-D2]	Δ[B3LYP-D3BJ]	Δ[BP86]	Δ[BP86-D2]	Δ[BP86-D3BJ]
Cu(1)···Cu(2)	3.392	0.006	0.047	–0.228	–0.247	0.368	–0.155	–0.176	0.224	–0.257	–0.330
Cu(1)–P(2)	2.238	0.039	0.030	–0.004	0.005	0.066	0.020	0.030	0.024	–0.019	–0.010
Cu(2)–P(1)	2.253	0.029	0.020	–0.018	–0.008	0.062	0.013	0.020	0.016	–0.023	–0.019
Cu(1)–P(3)	2.254	0.028	0.017	–0.021	–0.008	0.061	0.009	0.017	0.016	–0.024	0.080
Cu(2)–P(4)	2.257	0.020	0.010	–0.029	–0.017	0.046	0.000	0.010	0.003	–0.035	–0.033
Cu(1)–B(1)	2.195	0.001	0.000	–0.019	–0.010	0.044	0.011	0.021	0.007	–0.025	–0.011
Cu(2)–B(2)	2.191	0.005	0.004	–0.016	–0.008	0.049	0.023	0.023	0.012	–0.011	–0.009
Cu(1)–H(1)BA	1.768	0.008	0.006	–0.014	–0.012	0.042	0.004	–0.001	0.013	–0.021	–0.022
Cu(1)–H(1)BB	1.896	–0.057	–0.077	–0.086	–0.073	–0.048	–0.070	–0.046	–0.080	–0.101	–0.073
B(1)–H(1)BA	1.12	0.158	0.166	0.166	0.165	0.151	0.151	0.150	0.167	0.168	0.165
B(1)–H(1)BB	1.12	0.150	0.160	0.160	0.158	0.145	0.148	0.142	0.160	0.163	0.157
B(1)–H(1)BC	1.12	0.087	0.095	0.095	0.095	0.086	0.085	0.085	0.094	0.093	0.094
B(1)–H(1)BD	1.12	0.087	0.095	0.096	0.095	0.086	0.087	0.086	0.095	0.095	0.095
Cu(2)– H(2)BA	1.9398	–0.101	–0.116	–0.134	–0.120	–0.088	–0.089	–0.095	–0.117	–0.125	–0.123
Cu(2)– H(2)BB	1.6944	0.082	0.079	0.061	0.061	0.113	0.081	0.073	0.086	0.065	0.051
B(2)–H(2)BA	1.12	0.150	0.159	0.161	0.158	0.144	0.143	0.143	0.159	0.158	0.158
B(2)–H(2)BB	1.119	0.159	0.167	0.167	0.166	0.152	0.152	0.151	0.168	0.165	0.166
B(2)–H(2)BC	1.12	0.087	0.095	0.095	0.095	0.086	0.087	0.085	0.095	0.096	0.094
B(2)–H(2)BD	1.12	0.087	0.095	0.096	0.095	0.086	0.088	0.086	0.095	0.097	0.095
H(1)BB···H(2)BA	3.1143	–0.205	–0.024	–0.392	–0.401	0.608	–0.441	–0.278	0.308	–0.650	–0.540
B(1)···B(2)	5.06(1)	0.302	0.456	–0.844	0.114	1.084	0.004	0.232	0.786	–0.181	–0.01

Angles,°	1	Δ[M06]	Δ[PBE0]	Δ[PBE0-D2]	Δ[PBE0-D3BJ]	Δ[B3LYP]	Δ[B3LYP-D2]	Δ[B3LYP-D3BJ]	Δ[BP86]	Δ[BP86-D2]	Δ[BP86-D3BJ]
P(2)–Cu(1)–P(3)	112.94	–1.36	5.13	5.13	0.52	8.14	2.95	–0.91	7.29	2.50	–2.37
H(1)BA–Cu(1)–H(1)BB	60.95	9.65	10.32	10.32	10.59	7.78	9.20	8.58	10.05	11.52	10.64
P(1)–Cu(2)–P(4)	111.34	0.25	7.01	7.01	1.87	9.63	4.05	0.33	9.89	3.10	–1.19
H(2)BA–Cu(2)–H(2)BB	60.84	9.76	10.35	10.35	10.76	7.86	8.61	8.78	10.01	10.75	10.94
P(1)–C(1)–P(2)	112.6	–3.61	–1.54	–1.54	–1.54	1.26	–4.27	–4.76	–0.24	–6.17	–7.17
P(3)–C(2)–P(4)	109.9	–0.91	1.06	1.06	1.06	4.19	–1.05	–2.26	2.61	–3.08	–4.57
Cu(1)–H(1)BA–B(1)	96.3	–5.85	–6.09	–6.09	–6.09	–4.76	–4.89	–4.06	–6.03	–6.34	–5.38
Cu(1)–H(1)BB–B(1)	89.6	–1.70	–1.17	–1.17	–1.17	0.39	–0.49	–0.92	–0.68	–1.56	–1.86
Cu(2)–H(2)BA–B(2)	87.1	0.80	1.14	1.14	1.14	2.75	1.40	1.67	1.59	0.74	0.75
Cu(2)–H(2)BB–B(2)	100.2	–9.74	–9.92	–9.92	–9.92	–8.54	–8.49	–8.08	–9.82	–10.07	–9.38
Dihedral Angles,°	1	Δ[M06]	Δ[PBE0]	Δ[PBE0-D2]	Δ[PBE0-D3BJ]	Δ[B3LYP]	Δ[B3LYP-D2]	Δ[B3LYP-D3BJ]	Δ[BP86]	Δ[BP86-D2]	Δ[BP86-D3BJ]
χ_1(P,Cu,Cu,P)	–92.42	4.79	–0.23	8.51	7.99	–7.39	4.39	8.59	–2.72	5.64	8.55
χ_2(P,Cu,Cu,P)	133.70	3.39	12.42	10.58	9.66	13.98	11.14	7.65	14.41	10.55	3.71

Table S4. Structural parameters of crystal structure **2 (**Boat-Boat**)** and optimized structures.

Distances, Å	**2**	**M06**	**PBE0**	**PBE0-D2**	**PBE0-D3BJ**	**B3LYP**	**B3LYP-D2**	**B3LYP-D3BJ**	**BP86**	**BP86-D2**	**BP86-D3BJ**
Cu(1)–Cu(2)	3.2035(4)	3.298	3.462	3.181	3.183	3.689	3.244	3.225	3.540	3.146	3.018
Cu(1)–P(2)	2.2234(7)	2.277	2.267	2.227	2.238	2.318	2.255	2.264	2.273	2.220	2.224
Cu(2)–P(1)	2.2608(7)	2.282	2.255	2.234	2.247	2.305	2.260	2.274	2.262	2.228	2.233
Cu(1)–P(3)	2.2288(6)	2.282	2.260	2.235	2.244	2.309	2.264	2.272	2.265	2.228	2.233
Cu(2)–P(4)	2.2542(6)	2.277	2.261	2.226	2.238	2.313	2.254	2.265	2.269	2.214	2.224
Cu(1)–B(1)	2.198(2)	2.196	2.194	2.179	2.181	2.238	2.214	2.212	2.202	2.179	2.184
Cu(2)–B(2)	2.192(3)	2.196	2.191	2.174	2.182	2.239	2.207	2.213	2.202	2.170	2.184
Cu(1)–H(1)BA	1.79(2)	1.839	1.816	1.816	1.814	1.850	1.847	1.843	1.818	1.814	1.823
Cu(1)–H(1)BB	1.78(3)	1.776	1.779	1.762	1.756	1.807	1.775	1.768	1.781	1.757	1.748
B(1)–H(1)BA	1.15(2)	1.270	1.280	1.279	1.280	1.265	1.264	1.263	1.280	1.279	1.277
B(1)–H(1)BB	1.18(3)	1.278	1.286	1.284	1.286	1.271	1.270	1.270	1.287	1.284	1.284
B(1)–H(1)BC	1.11(3)	1.207	1.215	1.216	1.214	1.206	1.207	1.205	1.214	1.215	1.214
B(1)–H(1)BD	1.12(3)	1.207	1.215	1.216	1.215	1.206	1.208	1.206	1.215	1.217	1.215
Cu(2)–H(2)BA	1.75(3)	1.776	1.775	1.754	1.759	1.807	1.773	1.769	1.780	1.795	1.748
Cu(2)–H(2)BD	1.77(2)	1.839	1.820	1.804	1.818	1.854	1.827	1.845	1.824	1.747	1.823
B(2)–H(2)BA	1.21(3)	1.278	1.286	1.287	1.285	1.270	1.271	1.270	1.286	1.288	1.284
B(2)–H(2)BD	1.21(2)	1.270	1.279	1.281	1.279	1.264	1.268	1.263	1.279	1.283	1.277
B(2)–H(2)BC	1.15(3)	1.207	1.216	1.216	1.215	1.207	1.207	1.206	1.215	1.213	1.214
B(2)–H(2)BB	1.10(3)	1.207	1.215	1.213	1.215	1.206	1.205	1.205	1.215	1.215	1.215
H(1)BB···H(2)BA	2.59(4)	2.909	3.127	2.582	2.701	3.582	2.675	2.833	3.252	2.468	2.516
B(1)–B(2)	4.731(4)	5.363	5.561	4.995	5.166	5.999	5.068	5.289	5.687	4.873	4.966
H(10)A···Cl(2)D	3.031	–	–	–	–	–	–	–	–	–	–
H(26)A···H(1)BD	2.246	–	–	–	–	–	–	–	–	–	–

Angles,°	2	M06	PBE0	PBE0-D2	PBE0-D3BJ	B3LYP	B3LYP-D2	B3LYP-D3BJ	BP86	BP86-D2	BP86-D3BJ
P(2)–Cu(1)–P(3)	117.74(2)	111.584	119.267	115.259	112.483	120.928	115.194	111.462	120.293	113.400	110.522
H(1)BA–Cu(1)–H(1)BB	64(1)	70.604	71.239	71.598	71.809	68.719	69.507	69.695	70.959	71.669	71.512
P(1)–Cu(2)–P(4)	117.29(2)	111.590	117.354	116.085	112.909	120.358	116.110	111.636	119.647	115.233	110.522
H(2)BA–Cu(2)–H(2)BD	67(1)	70.604	71.291	72.236	71.618	68.636	70.107	69.614	70.845	72.498	71.512
P(1)–C(1)–P(2)	110.6(1)	108.993	110.837	107.498	107.108	113.429	108.813	107.714	111.939	106.592	105.229
P(3)–C(2)–P(4)	111.5(1)	108.991	111.432	107.351	107.242	113.684	108.421	107.772	112.150	106.688	105.230
Cu(1)–H(1)BA–B(1)	94(1)	87.904	88.461	87.690	87.866	89.839	88.675	88.767	88.822	87.798	87.737
Cu(1)–H(1)BB–B(1)	94(2)	90.455	89.931	89.908	90.222	91.587	91.712	91.967	90.242	90.179	90.836
Cu(2)–H(2)BA–B(2)	94(2)	90.461	89.937	89.907	90.223	91.683	91.435	91.984	90.372	89.984	90.836
Cu(2)–H(2)BD–B(2)	93(1)	87.901	88.145	87.852	87.822	89.731	89.064	88.754	88.622	88.030	87.737
C(10)–H(10)A···Cl(2)D	149.2	–	–	–	–	–	–	–	–	–	–
C(26)–H(26)A···H(1)BD	168.2	–	–	–	–	–	–	–	–	–	–
Dihedral Angles,°	2	M06	PBE0	PBE0-D2	PBE-D3BJ	B3LYP	B3LYP-D2	B3LYP-D3BJ	BP86	BP86-D2	BP86-D3BJ
χ_1(P,Cu,Cu,P)	117.04(2)	87.432	146.479	87.452	84.979	148.891	87.925	84.165	148.106	86.633	84.404
χ_2(P,Cu,Cu,P)	−118.44(2)	−137.150	−92.806	–145.202	−141.616	–97.280	–145.005	–140.400	–95.140	–143.184	–136.953

Table S5. Energy of the formation of the DFT-optimized geometries' binuclear complexes (**1** and **2**) computed relative to the monomer complexes.

Energy, kcal/mol	M06/1	M06/2	PBE0 /1	PBE0 /2	PBE0-D2/1	PBE0-D2/2	PBE0-D3BJ/1	PBE0-D3BJ/2	B3LYP /1	B3LYP /2	B3LYP-D2/1	B3LYP-D2/2	B3LYP-D3BJ/1	B3LYP-D3BJ/1	BP86 /1	BP86 /2	BP86-D2/1	BP86-D2/2	BP86-D3BJ/1	BP86-D3BJ/2
ΔE	−45.8	−46.0	−31.7	−31.7	−54.7	−54.6	−60.5	−60.5	−20.2	−19.8	−49.6	−49.7	−58.5	−58.5	−25.3	−25.1	−57.5	−57.7	–71.4	–71.3
ΔE_{ZPE}	−42.7	−42.5	−29.8	−29.4	−52.6	−52.5	−57.6	−57.6	−18.2	−17.9	−47.4	−47.5	−55.8	−56.0	−23.2	−22.9	−55.2	−55.3	–69.1	–69.3
$\Delta H°$	−43.4	−43.3	−30.2	−30.0	−52.9	−52.9	−58.4	−58.4	−18.5	−18.2	−47.6	−47.7	−56.2	−56.3	−23.7	−23.5	−55.6	−55.8	–68.2	–68.3
$\Delta G°$	−23.3	−22.8	−11.2	−9.5	−35.7	−34.3	−37.3	−36.8	2.1	2.2	−30.1	−29.9	−51.8	−51.8	−2.9	−2.5	−36.7	−36.1	–54.9	–54.4
ΔE_{DCM}	−41.8	−41.7	−25.9	−25.9	−48.1	−48.2	−52.3	−52.4	−14.2	−13.4	−43.5	−43.5	−49.4	−49.6	−18.7	−18.1	−50.9	−51.0	–64.9	–65.1
$\Delta H°_{DCM}$	−39.4	−39.1	−24.3	−24.2	−46.3	−46.5	−50.2	−50.3	−12.5	−11.8	−41.5	−41.5	−27.2	−28.2	−17.1	−16.5	−49.0	−49.1	–61.7	–62.2
$\Delta G°_{DCM}$	−19.3	−18.6	−5.4	−3.8	−29.1	−27.9	−37.3	−36.8	8.1	8.6	−24.0	−23.7	−34.0	−34.9	3.8	4.5	−30.1	−29.5	–48.4	–48.3

Table S6. CCDC analysis of the structures, containing {Cu(BH_4)} moieties.

CSD refcode	Complex	BH ligand	Cu-B	Cu-H	XCuX	X	Ref
EXEJAU	(μ_3-H)-(μ_3-BH_4)(μ_2-PPh_2NHPPh_2)$_3Cu_3$	η^1	2.549 2.584 2.598	1.841 1.836 1.949	–	P	[80]
POSCAB	[(EtO)$_3$P](phen)Cu(η^2-BH_4)	η^2	2.341	1.981 2.161	78.34	N	[81]
ALUDUH	{C[(Fe(CO)$_3$]$_4$}Cu(η^2-BH_4)	η^2	2.140	1.756 1.728	–	Fe	[82]
BAWNAO	(PPh_3)(phen)Cu(η^2-BH_4)	η^2	2.274	1.406	78.11	N	[83]
BAWNAO01	(PPh_3)(phen)Cu(η^2-BH_4)	η^2	2.320	1.571	77.60	N	[84]
BAWNAO02	(PPh_3)(phen)Cu(η^2-BH_4)	η^2	2.290	1.733 2.079	77.86	N	[84]
BHTPCU11	(PPh_3)$_2$Cu(η^2-BH_4) T=295K	η^2	2.252	1.731 1.731	122.79	P	[84]
BHTPCU12	(PPh_3)$_2$Cu(η^2-BH_4) T=90K	η^2	2.212	1.790 1.790	122.99	P	[85]
BHTPCU13	(PPh_3)$_2$Cu(η^2-BH_4) T=90K	η^2	2.212	1.809 1.809	123.01	P	[86]
DAYHEQ	(PPh_3)$_2$Cu(η^2-BH_4) · Py	η^2	2.189	1.74 1.860	123.01	P	[87]
CICFID	[{(PPh_3)$_2$Cu}$_2$(μ,η^2:η^2-BH_4)][ClO_4]	μ,η^2:η^2	2.232 2.204	1.812 1.863	119.66 124.51	P	[88]
CIFSUF	(2,9-Me-4,7-Ph-phen)Cu(η^2-BH_4) T=295K	η^2	2.112	–	–	N	[84]
CIFSUF01	(2,9-Me-4,7-Ph-phen)Cu(η^2-BH_4) T=90K	η^2	2.115	1.669 1.651	–	N	[89]
LESPIJ	(PPh_3)(4,7-Me-phen)Cu(η^2-BH_4) T=200K	η^2	2.286	2.027 1.676	–	N	[90]
CIGQIU	[(*p*-MeOPh)$_3$P]$_2$Cu(η^2-BH_4)	η^2	2.180	1.859 1.859	121.51	P	[91]
CIGQOA	(PCy_3)$_2$Cu(η^2-BH_4)	η^2	2.234	1.813	132.45	P	[91]
CIGQUG	[CH_3Ph)$_3$P]$_2$Cu(η^2-BH_4)	η^2	2.185	1.754 1.735	119.9	P	[91]
COJMIX	(^{n}BuPPh$_2$)$_2$Cu(η^2-BH_4)	η^2	2.190	1.601 1.801	113.97	P	[92]
NOKLAC	[(NCEt)$_3$P]$_2$Cu(η^2-BH_4)	η^2	2.222	1.831 1.847	125.7	P	[93]
PHRLCU	(Dmphen)Cu(η^2-BH_4)	η^2	2.079	1.579 1.579	81.73	N	[94]
SUFJUA	(CAAC)Cu(η^2-BH_4)	η^2	2.101	1.679 1.717	–	C	[95]
TUFBOL	($FcPPh_2$)$_2$Cu(η_2-BH_4)	η^2	2.158	1.654 1.600	112.69	P	[96]
VUDKUA	[{$Ph_2P(CH_2)_2$}$_2$$NCH_2$]$_2$Cu($\eta^2$-$BH_4$)	η^2	2.247 2.247	1.691 1.675 1.691 1.675	119.72 119.72	P	[97]
BOLJAN	(triphos)Cu(η^1-BH_4)	η^1	2.441	1.605	–	P	[98]
TMPCUB01	[($MePh_2CH_3$)$_3$P]$_3$Cu(η^1-BH_4) T=15K	η^1	3.128	1.698	–	P	[99]
TMPCUB02	[($MePh_2CH_3$)$_3$P]$_3$Cu(η^1-BH_4) T=295K	η^1	2.578	1.835	–	P	[99]
TMPCUB03	[($MePh_2CH_3$)$_3$P]$_3$Cu(η^1-BH_4) T=295K	η^1	2.499	–	–	P	[99]
TMPCUB10	[($MePh_2CH_3$)$_3$P]$_3$Cu(η^1-BH_4)	η^1	2.646	1.467	–	P	[100,101]
HAFSUC	(cyclam)Cu(η^1-BH_4)	η^1	3.093	2.274	–	N	[102]

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Table S7. DFT-optimised geometries (Cartesian coordinates) and electronic energies.

55

M06/(dppm)Cu(BH$_4$) E= -3315.14655316 Ha

29	-1.400396000	1.049921000	1.963463000
15	1.595006000	-0.725309000	1.256563000
15	-1.253838000	-0.224446000	0.173295000
6	0.204674000	-1.369847000	0.165906000
1	0.547785000	-1.550064000	-0.862439000
1	-0.138227000	-2.327291000	0.581910000
5	-1.596316000	2.324191000	3.636092000
1	-1.933052000	2.656226000	2.443361000
1	-1.265380000	1.083258000	3.702378000
1	-0.632007000	2.976993000	3.944184000
1	-2.564483000	2.463447000	4.328611000
6	1.739295000	0.988508000	0.597343000
6	1.382115000	2.040508000	1.455479000
6	2.097878000	1.283668000	-0.728188000
6	1.358798000	3.359544000	0.992511000
6	2.087350000	2.598899000	-1.185697000
6	1.710832000	3.637064000	-0.326981000
1	1.124557000	1.831616000	2.493557000
1	2.383313000	0.476947000	-1.401820000
1	1.060086000	4.155766000	1.668695000
1	2.356587000	2.816014000	-2.216142000
1	1.694228000	4.661173000	-0.690059000
6	3.040004000	-1.535905000	0.454121000
6	4.304591000	-0.935370000	0.583786000
6	2.955370000	-2.782254000	-0.184050000
6	5.443009000	-1.552707000	0.072404000
6	4.097851000	-3.401740000	-0.694609000
6	5.343052000	-2.788197000	-0.570863000
1	4.391745000	0.029958000	1.078887000
1	1.995272000	-3.283894000	-0.284681000
1	6.410584000	-1.069200000	0.175374000
1	4.011360000	-4.365538000	-1.189247000
1	6.231469000	-3.269503000	-0.969648000
6	-2.660689000	-1.372042000	-0.057946000
6	-3.356426000	-1.518833000	-1.264042000
6	-3.058716000	-2.123610000	1.060298000
6	-4.422774000	-2.415337000	-1.353353000
6	-4.117706000	-3.022862000	0.964980000
6	-4.800900000	-3.170028000	-0.243984000
1	-3.074640000	-0.927497000	-2.131408000
1	-2.544580000	-1.991309000	2.012347000
1	-4.959204000	-2.520074000	-2.292161000
1	-4.417800000	-3.598204000	1.835842000
1	-5.632394000	-3.865078000	-0.316731000
6	-1.118779000	0.716498000	-1.383748000
6	-1.448555000	2.078429000	-1.369056000
6	-0.696339000	0.129866000	-2.587539000
6	-1.347708000	2.842535000	-2.532154000
6	-0.594868000	0.893802000	-3.747435000
6	-0.918038000	2.252703000	-3.719868000
1	-1.765593000	2.544963000	-0.437214000
1	-0.446063000	-0.929178000	-2.623713000
1	-1.598392000	3.898868000	-2.504999000
1	-0.264230000	0.431083000	-4.672999000
1	-0.835329000	2.848412000	-4.624511000

110

M06/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6630.36616569 Ha

29	-0.002785000	1.644781000	-1.227336000
29	-0.001729000	-1.639445000	-1.231047000
15	-2.101712000	-1.313054000	-0.402897000
15	-1.581100000	1.541564000	0.411490000
15	2.099356000	1.314181000	-0.404166000
15	1.570946000	-1.540208000	0.414070000
5	-0.199357000	2.672455000	-3.160269000
1	-0.334039000	1.417964000	-2.956913000
1	-1.209781000	3.045333000	-3.705203000
1	0.811401000	2.852112000	-3.794755000
1	-0.111281000	3.287414000	-2.052757000
5	0.208628000	-2.668454000	-3.160349000
1	1.227597000	-3.022253000	-3.702110000
1	-0.797459000	-2.871721000	-3.794953000
1	0.132798000	-3.281099000	-2.050206000
1	0.314688000	-1.409933000	-2.962499000
6	-2.132356000	-0.122260000	1.014524000
1	-1.399264000	-0.509814000	1.739188000
1	-3.114068000	-0.054523000	1.503723000
6	2.113475000	0.127204000	1.017497000
1	3.085866000	0.058378000	1.524841000
1	1.368935000	0.518240000	1.729060000
6	-2.792141000	-2.844361000	0.322975000
6	-3.236093000	-2.961763000	1.645762000
1	-3.190655000	-2.110207000	2.321459000
6	-3.715431000	-4.183433000	2.122635000
1	-4.052422000	-4.263722000	3.153009000
6	-3.754708000	-5.296257000	1.283972000
1	-4.129901000	-6.245753000	1.655897000
6	-3.306624000	-5.189408000	-0.035394000
1	-3.329156000	-6.054882000	-0.691319000
6	-2.825565000	-3.973415000	-0.513669000
1	-2.463885000	-3.894307000	-1.538956000
6	-3.436749000	-0.711499000	-1.491892000
6	-4.757633000	-0.576629000	-1.034653000
1	-5.014292000	-0.861595000	-0.014828000
6	-5.744185000	-0.087136000	-1.885128000
1	-6.764219000	0.021609000	-1.526982000
6	-5.419084000	0.269786000	-3.197599000
1	-6.190142000	0.654522000	-3.859587000
6	-4.111718000	0.132155000	-3.659729000
1	-3.856512000	0.407927000	-4.678344000
6	-3.118974000	-0.363085000	-2.811126000
1	-2.098617000	-0.482333000	-3.171508000
6	-3.153688000	2.432027000	0.139761000
6	-4.111102000	2.556500000	1.158334000
1	-3.912612000	2.143342000	2.147104000
6	-5.309388000	3.221703000	0.916038000
1	-6.049042000	3.315219000	1.706535000
6	-5.554670000	3.777522000	-0.343297000
1	-6.489902000	4.297738000	-0.531678000
6	-4.600989000	3.670670000	-1.353462000
1	-4.787322000	4.104508000	-2.331492000
6	-3.398337000	2.999769000	-1.116758000
1	-2.656885000	2.907836000	-1.910028000
6	-0.897302000	2.362105000	1.903503000
6	-0.763236000	1.765617000	3.164763000
1	-1.152270000	0.766163000	3.350821000
6	-0.130251000	2.450109000	4.206664000
1	-0.030582000	1.974539000	5.179214000
6	0.359488000	3.739583000	4.004620000
1	0.852635000	4.268887000	4.815228000
6	0.215497000	4.348933000	2.755726000
1	0.603954000	5.349344000	2.586831000
6	-0.397850000	3.663198000	1.711562000
1	-0.482803000	4.133291000	0.731498000
6	2.807798000	2.839647000	0.315485000
6	2.863637000	3.962012000	-0.529012000
1	2.509632000	3.880045000	-1.556797000
6	3.356443000	5.174918000	-0.055096000
1	3.396355000	6.035308000	-0.716857000
6	3.793066000	5.285540000	1.267876000
1	4.176711000	6.232893000	1.636603000
6	3.731284000	4.179524000	2.114121000
1	4.059546000	4.262954000	3.147056000
6	3.240857000	2.960612000	1.641443000
1	3.178252000	2.114527000	2.322616000
6	3.419787000	0.691926000	-1.499351000
6	4.725794000	0.472376000	-1.032456000
1	4.988851000	0.724720000	-0.005780000
6	5.685869000	-0.076148000	-1.876344000
1	6.690221000	-0.263246000	-1.506164000
6	5.354445000	-0.391669000	-3.198027000
1	6.104961000	-0.823019000	-3.855012000
6	4.067757000	-0.151585000	-3.675867000
1	3.808378000	-0.392327000	-4.702282000
6	3.097910000	0.390541000	-2.829239000
1	2.090085000	0.574055000	-3.197438000
6	3.154551000	-2.412965000	0.146620000
6	4.092650000	-2.562111000	1.179977000
1	3.861574000	-2.203640000	2.182822000
6	5.316081000	-3.178040000	0.932311000
1	6.039974000	-3.291816000	1.734674000
6	5.608211000	-3.655932000	-0.348993000
1	6.563895000	-4.135865000	-0.541944000
6	4.673787000	-3.525719000	-1.374190000
1	4.895266000	-3.900369000	-2.369327000
6	3.445324000	-2.906758000	-1.130966000
1	2.713862000	-2.806866000	-1.932337000
6	0.889751000	-2.362173000	1.905662000
6	0.749324000	-1.762710000	3.164886000
1	1.131888000	-0.760263000	3.348272000
6	0.118692000	-2.448101000	4.207589000
1	0.014197000	-1.970417000	5.178599000
6	-0.362480000	-3.741219000	4.008275000
1	-0.854314000	-4.271111000	4.819307000
6	-0.212131000	-4.353365000	2.761500000
1	-0.595633000	-5.355963000	2.593956000
6	0.399445000	-3.667072000	1.716620000
1	0.488322000	-4.138781000	0.737748000

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M06/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6630.36633635 Ha

29	-0.006509000	-1.649044000	-1.228961000
29	0.006510000	1.648792000	-1.228952000
15	-1.577910000	-1.536976000	0.415028000
15	-2.095766000	1.320844000	-0.404570000
15	2.095751000	-1.320825000	-0.404525000
15	1.578033000	1.537021000	0.415017000
6	3.417638000	-0.701711000	-1.499953000
6	-3.417689000	0.701819000	-1.500005000
6	-3.240655000	2.967776000	1.639419000
1	-3.186734000	2.119634000	2.318789000
6	-0.896116000	-2.358457000	1.906656000
6	-3.164170000	-2.405624000	0.150075000
6	-2.116205000	0.132792000	1.016477000
1	-1.373946000	0.521855000	1.731325000
1	-3.090552000	0.066413000	1.520353000
6	-2.799525000	2.848114000	0.315979000
6	3.164340000	2.405586000	0.150122000
6	2.116185000	-0.132785000	1.016543000
1	1.373868000	-0.521759000	1.731383000
1	3.090520000	-0.066508000	1.520461000
6	-3.457394000	-2.899879000	-1.126775000
6	-4.102120000	-2.550538000	1.184181000
1	-3.869326000	-2.191507000	2.186439000
5	-0.220158000	-2.672475000	-3.160475000
6	3.240394000	-2.967913000	1.639419000
1	3.186348000	-2.119813000	2.318838000
6	2.799517000	-2.848140000	0.315905000
6	-3.096037000	0.397879000	-2.829377000
1	-2.087687000	0.578462000	-3.197636000
6	3.776514000	-5.297120000	1.268920000
1	4.157082000	-6.245623000	1.637883000
6	-4.724301000	0.485598000	-1.033220000
1	-4.987250000	0.739995000	-0.007031000
6	-5.327593000	-3.163040000	0.938115000
1	-6.051235000	-3.273708000	1.741134000
6	-0.759760000	-1.760760000	3.167163000
1	-1.146741000	-0.760220000	3.351783000
6	-5.685268000	-0.062252000	-1.876538000
1	-6.690055000	-0.246891000	-1.506305000
6	-3.727282000	4.188112000	2.112333000
1	-4.061934000	4.270506000	3.143298000
6	0.759762000	1.760998000	3.167115000
1	1.146785000	0.760496000	3.351849000
6	-2.842759000	3.973363000	-0.525384000
1	-2.482011000	3.892400000	-1.550944000
6	-4.066748000	-0.143602000	-3.675443000
1	-3.807631000	-0.386350000	-4.701448000
6	-5.354049000	-0.380431000	-3.197629000
1	-6.105181000	-0.811408000	-3.854150000
5	0.220257000	2.672263000	-3.160465000
6	0.896164000	2.358584000	1.906563000
6	0.360229000	-3.735852000	4.007854000
1	0.853556000	-4.265057000	4.818419000
6	3.095981000	-0.397686000	-2.829298000
1	2.087626000	-0.578262000	-3.197565000
6	-0.126879000	-2.445200000	4.209109000
1	-0.025128000	-1.968768000	5.181020000
6	-4.687982000	-3.515253000	-1.368429000
1	-4.911381000	-3.890231000	-2.363009000
6	-3.776736000	5.297010000	1.268998000
1	-4.157397000	6.245472000	1.637966000
6	2.842901000	-3.973318000	-0.525545000
1	2.482347000	-3.892273000	-1.551164000
6	-0.399911000	-3.660874000	1.715684000
1	-0.486280000	-4.131369000	0.735986000
6	0.399906000	3.660957000	1.715433000
1	0.486349000	4.131376000	0.735705000
6	3.331516000	-5.187820000	-0.051338000
1	3.361737000	-6.050406000	-0.710743000
6	0.213385000	-4.346556000	2.759961000
1	0.600291000	-5.347664000	2.591479000
6	3.726892000	-4.188297000	2.112341000
1	4.061332000	-4.270777000	3.143368000
6	0.126792000	2.445519000	4.208956000
1	0.025035000	1.969194000	5.180919000
6	-0.360417000	3.736110000	4.007527000
1	-0.853861000	4.265348000	4.817999000
6	-0.213555000	4.346690000	2.759579000
1	-0.600608000	5.347716000	2.590920000
6	-3.331470000	5.187829000	-0.051177000
1	-3.361569000	6.050466000	-0.710520000
6	4.724262000	-0.485545000	-1.033163000
1	4.987211000	-0.740058000	-0.007002000
6	-5.622080000	-3.641482000	-0.342448000
1	-6.579337000	-4.118752000	-0.534177000
6	5.685225000	0.062360000	-1.876445000
1	6.690025000	0.246938000	-1.506222000
6	5.353988000	0.380654000	-3.197506000
1	6.105113000	0.811685000	-3.854001000
6	4.066687000	0.143857000	-3.675332000
1	3.807571000	0.386668000	-4.701324000
6	3.457502000	2.900025000	-1.126672000
1	2.726449000	2.803221000	-1.928817000
6	4.102358000	2.550291000	1.184195000
1	3.869598000	2.191135000	2.186416000
6	5.622289000	3.641362000	-0.342375000
1	6.579567000	4.118594000	-0.534090000
6	5.327857000	3.162737000	0.938134000
1	6.051563000	3.273243000	1.741119000
6	4.688113000	3.515363000	-1.368310000
1	4.911467000	3.890490000	-2.362845000
1	-1.238330000	-3.030753000	-3.700709000
1	0.785791000	-2.868354000	-3.797855000
1	-0.334015000	-1.415683000	-2.958986000
1	-0.137264000	-3.287909000	-2.052144000
1	-0.785586000	2.867918000	-3.798060000
1	0.137145000	3.287762000	-2.052220000
1	0.334231000	1.415447000	-2.958788000
1	1.238490000	3.030541000	-3.700581000

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PBE0/(dppm)Cu(BH$_4$) E= -3314.11480323 Ha

29	-1.619314000	0.754527000	1.852656000
15	1.475176000	-0.705702000	1.146405000
15	-1.317725000	-0.210552000	-0.080363000
6	0.245726000	-1.235978000	-0.188801000
1	0.675181000	-1.188840000	-1.206000000
1	-0.041553000	-2.282656000	0.019409000
5	-1.956791000	1.731279000	3.680147000
1	-2.180151000	2.265632000	2.525050000
1	-1.622110000	0.487228000	3.569988000
1	-1.028364000	2.320981000	4.191831000
1	-3.002193000	1.759620000	4.287129000
6	1.786759000	1.060166000	0.676178000
6	1.381371000	2.057749000	1.596248000
6	2.372791000	1.457112000	-0.550581000
6	1.540926000	3.422442000	1.287124000
6	2.534923000	2.818568000	-0.853945000
6	2.115251000	3.802937000	0.062590000
1	0.943410000	1.767591000	2.557446000
1	2.711110000	0.698640000	-1.263147000
1	1.216535000	4.178999000	2.006780000
1	2.985774000	3.113735000	-1.806065000
1	2.242107000	4.862577000	-0.177668000
6	3.015141000	-1.533335000	0.533578000
6	4.276355000	-0.987976000	0.885760000
6	2.989259000	-2.767939000	-0.159397000
6	5.466873000	-1.648307000	0.543140000
6	4.183642000	-3.428812000	-0.499224000
6	5.425985000	-2.871734000	-0.151434000
1	4.322981000	-0.036248000	1.423596000
1	2.035243000	-3.224622000	-0.438102000
1	6.428664000	-1.206343000	0.819408000
1	4.140100000	-4.379970000	-1.038162000
1	6.353908000	-3.386090000	-0.416284000
6	-2.641748000	-1.431632000	-0.491363000
6	-3.450096000	-1.349612000	-1.646646000
6	-2.876595000	-2.471949000	0.442136000
6	-4.461428000	-2.302117000	-1.871238000
6	-3.881213000	-3.423908000	0.208575000
6	-4.675604000	-3.341723000	-0.950405000
1	-3.294801000	-0.543244000	-2.367742000
1	-2.283549000	-2.526290000	1.361756000
1	-5.082437000	-2.227167000	-2.768384000
1	-4.052082000	-4.221134000	0.937153000
1	-5.463283000	-4.078941000	-1.128276000
6	-1.227897000	0.932102000	-1.518481000
6	-1.541009000	2.294919000	-1.313214000
6	-0.854070000	0.497830000	-2.813399000
6	-1.478302000	3.207553000	-2.380927000
6	-0.794640000	1.411906000	-3.878282000
6	-1.104920000	2.768136000	-3.662651000
1	-1.819256000	2.635538000	-0.310628000
1	-0.616041000	-0.555122000	-2.994293000
1	-1.716505000	4.260344000	-2.207574000
1	-0.505427000	1.066838000	-4.874977000
1	-1.053715000	3.478541000	-4.492519000

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PBE0/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6628.28015261 Ha

29	-2.912803000	6.633157000	-3.468762000
29	-0.659062000	6.036462000	-5.997397000
15	0.472631000	7.560624000	-4.762692000
15	-1.981195000	8.679942000	-3.261276000
15	-4.307303000	6.269463000	-5.215059000
15	-2.231214000	6.778465000	-7.439752000
5	-3.107487000	5.140422000	-1.871057000
1	-2.169317000	5.191729000	-2.749838000
1	-2.573144000	5.155431000	-0.779624000
1	-3.788075000	4.156730000	-2.083095000
1	-3.834282000	6.189358000	-1.964365000
5	0.313023000	4.069227000	-6.064930000
1	-0.008019000	3.104679000	-6.731082000
1	1.262055000	3.878387000	-5.331179000
1	0.581285000	5.024836000	-6.871810000
1	-0.709003000	4.386404000	-5.351232000
6	-0.501693000	9.095968000	-4.339010000
1	-0.878137000	9.491814000	-5.300458000
1	0.117310000	9.867458000	-3.845415000
6	-3.905267000	7.263844000	-6.744187000
1	-4.680453000	7.172218000	-7.526672000
1	-3.843916000	8.317591000	-6.414499000
6	1.920816000	8.225190000	-5.701080000
6	2.119099000	9.592654000	-5.997302000
1	1.402389000	10.344437000	-5.656906000
6	3.239200000	10.005654000	-6.743476000
1	3.380141000	11.068174000	-6.963251000
6	4.173049000	9.060338000	-7.200706000
1	5.043676000	9.383434000	-7.778509000
6	3.981787000	7.695062000	-6.913416000
1	4.701339000	6.952468000	-7.269336000
6	2.863851000	7.277097000	-6.174444000
1	2.710593000	6.212512000	-5.970264000
6	1.237846000	7.068912000	-3.158658000
6	2.095343000	7.944359000	-2.454049000
1	2.335675000	8.930404000	-2.860925000
6	2.654155000	7.547070000	-1.226129000
1	3.313630000	8.229566000	-0.682317000
6	2.367670000	6.271732000	-0.700638000
1	2.804905000	5.964409000	0.253806000
6	1.526646000	5.393847000	-1.404630000
1	1.302820000	4.401830000	-1.004031000
6	0.963353000	5.787071000	-2.632911000
1	0.319708000	5.100586000	-3.187815000
6	-1.398855000	9.167439000	-1.574803000
6	-1.036539000	10.500363000	-1.266902000
1	-1.128619000	11.284778000	-2.025210000
6	-0.583816000	10.831587000	0.020038000
1	-0.310517000	11.865360000	0.251511000
6	-0.492120000	9.836602000	1.012559000
1	-0.142016000	10.097021000	2.015700000
6	-0.859111000	8.513501000	0.714970000
1	-0.796463000	7.737580000	1.482711000
6	-1.314914000	8.175141000	-0.572861000
1	-1.610227000	7.145030000	-0.795693000
6	-3.170959000	10.037155000	-3.679651000
6	-2.811975000	11.238315000	-4.335922000
1	-1.777018000	11.414818000	-4.642425000
6	-3.780077000	12.223425000	-4.603876000
1	-3.486347000	13.145952000	-5.113273000
6	-5.117359000	12.025357000	-4.217753000
1	-5.868029000	12.792525000	-4.427801000
6	-5.486311000	10.835424000	-3.563953000
1	-6.525686000	10.665198000	-3.270731000
6	-4.522634000	9.848005000	-3.299534000
1	-4.819486000	8.916889000	-2.806185000
6	-6.034366000	6.794702000	-4.812538000
6	-6.648059000	6.177174000	-3.692740000
1	-6.098655000	5.422453000	-3.121203000
6	-7.948951000	6.537261000	-3.307456000
1	-8.409622000	6.050351000	-2.443416000
6	-8.654859000	7.522920000	-4.023923000
1	-9.667610000	7.802952000	-3.720446000
6	-8.051654000	8.145773000	-5.129711000
1	-8.593173000	8.912453000	-5.691943000
6	-6.749318000	7.784568000	-5.523705000
1	-6.296996000	8.285617000	-6.383448000
6	-4.560828000	4.559133000	-5.855871000
6	-5.526611000	4.280272000	-6.852449000
1	-6.161254000	5.082058000	-7.243505000
6	-5.682727000	2.972847000	-7.337003000
1	-6.426331000	2.764898000	-8.111699000
6	-4.884077000	1.931097000	-6.825396000
1	-5.007434000	0.912642000	-7.205094000
6	-3.935686000	2.198437000	-5.824211000
1	-3.316411000	1.393615000	-5.419916000
6	-3.773156000	3.508414000	-5.336101000
1	-3.044412000	3.716322000	-4.549218000
6	-2.685112000	5.653190000	-8.835269000
6	-3.457726000	6.097107000	-9.934631000
1	-3.775539000	7.143022000	-9.998027000
6	-3.798591000	5.206408000	-10.965098000
1	-4.391900000	5.558183000	-11.814320000
6	-3.369096000	3.866233000	-10.909379000
1	-3.633869000	3.174255000	-11.714221000
6	-2.593746000	3.422979000	-9.824809000
1	-2.252001000	2.385478000	-9.778080000
6	-2.246848000	4.311337000	-8.790080000
1	-1.634160000	3.964955000	-7.952292000
6	-1.700866000	8.321504000	-8.315701000
6	-2.568349000	9.388093000	-8.650964000
1	-3.629359000	9.344985000	-8.388088000
6	-2.078947000	10.522172000	-9.324872000
1	-2.762309000	11.338762000	-9.575875000
6	-0.720103000	10.605845000	-9.675732000
1	-0.342236000	11.488860000	-10.198818000
6	0.151948000	9.551596000	-9.347641000
1	1.213122000	9.611985000	-9.603697000
6	-0.332934000	8.420011000	-8.671069000
1	0.353899000	7.611085000	-8.402144000

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PBE0/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6628.28008304 Ha

29	6.039569000	3.545440000	2.277929000
29	5.654960000	6.794765000	3.409208000
15	3.848410000	3.550133000	2.860651000
15	4.010708000	5.996221000	4.729207000
15	7.609522000	3.300768000	3.884767000
15	7.786740000	6.385263000	4.042225000
6	9.271616000	2.707830000	3.331917000
6	2.391207000	6.879164000	4.655673000
6	4.984531000	5.106641000	7.302005000
1	5.051233000	4.090567000	6.902334000
6	3.166671000	1.832240000	2.917675000
6	2.612465000	4.430590000	1.811714000
6	3.493842000	4.199059000	4.575549000
1	4.098523000	3.584452000	5.265163000
1	2.429230000	4.101408000	4.853785000
6	4.466329000	6.165334000	6.519653000
6	9.138937000	6.395347000	2.789821000
6	8.043184000	4.778462000	4.957878000
1	7.337676000	4.799166000	5.809042000
1	9.074162000	4.680931000	5.344483000
6	3.062486000	5.244404000	0.748855000
1	4.131956000	5.325701000	0.542781000
6	1.223631000	4.308445000	2.056590000
1	0.862715000	3.660882000	2.862302000
6	6.341272000	3.232779000	0.127394000
6	7.463631000	2.102103000	6.517582000
1	8.058035000	2.937712000	6.898712000
6	7.117075000	2.036505000	5.146440000
6	2.166835000	7.803299000	3.611794000
1	2.957039000	8.002457000	2.880939000
6	6.287021000	0.008095000	6.944186000
1	5.965273000	-0.772456000	7.639318000
6	1.369652000	6.639134000	5.606607000
1	1.541940000	5.941318000	6.432764000
6	0.302157000	5.005258000	1.260187000
1	-0.769475000	4.908588000	1.456872000
6	2.598088000	1.239701000	4.068249000
1	2.513595000	1.804237000	5.000478000
6	0.140303000	7.309495000	5.507746000
1	-0.643031000	7.122250000	6.248166000
6	5.426375000	5.335905000	8.618823000
1	5.813554000	4.499479000	9.208634000
6	8.690205000	7.365996000	6.602861000

1	8.648281000	6.340943000	6.979861000
6	4.409518000	7.462062000	7.091672000
1	4.014786000	8.296501000	6.504864000
6	0.931043000	8.470761000	3.517157000
1	0.766837000	9.183591000	2.704594000
6	-0.080649000	8.225827000	4.460710000
1	-1.038786000	8.748433000	4.386382000
5	5.477665000	8.416255000	1.947031000
6	8.354769000	7.653044000	5.260401000
6	2.236733000	-0.842121000	2.849029000
1	1.876856000	-1.874573000	2.822468000
6	9.567970000	2.727541000	1.951013000
1	8.810794000	3.060704000	1.234703000
6	2.137155000	-0.090236000	4.031941000
1	1.697174000	-0.534001000	4.930070000
6	2.133852000	5.941450000	-0.046469000
1	2.493417000	6.574377000	-0.861791000
6	5.363573000	6.625044000	9.173925000
1	5.707493000	6.802188000	10.196718000
6	6.346683000	0.938190000	4.692692000
1	6.057657000	0.883020000	3.638145000
6	3.268429000	1.063349000	1.729846000
1	3.722344000	1.503354000	0.836173000
6	8.401079000	8.998405000	4.813678000
1	8.120877000	9.237567000	3.782886000
6	5.937788000	-0.068718000	5.583629000
1	5.335485000	-0.902654000	5.213508000
6	2.802491000	-0.260463000	1.698213000
1	2.886307000	-0.839567000	0.774386000
6	7.049052000	1.094982000	7.408758000
1	7.326146000	1.158943000	8.465310000
6	9.073360000	8.399672000	7.477915000
1	9.328886000	8.162343000	8.514886000
6	9.128990000	9.727701000	7.023443000
1	9.429035000	10.529197000	7.704494000
6	8.791309000	10.023617000	5.688915000
1	8.825229000	11.055875000	5.329461000
6	4.853416000	7.686942000	8.404184000
1	4.802459000	8.694983000	8.824838000
6	10.249602000	2.252352000	4.247596000
1	10.022649000	2.203156000	5.317517000
6	0.757391000	5.825509000	0.209305000
1	0.037501000	6.368262000	-0.410182000
6	11.509220000	1.835878000	3.788138000
1	12.258263000	1.480117000	4.501801000
6	11.803768000	1.868465000	2.411379000
1	12.785259000	1.541967000	2.055359000
6	10.833509000	2.311786000	1.497126000
1	11.053073000	2.333890000	0.426328000
6	8.801960000	6.445736000	1.419013000
1	7.752404000	6.505285000	1.121075000
6	10.501063000	6.347517000	3.171419000
1	10.774202000	6.333514000	4.231578000
6	11.165283000	6.371580000	0.827744000
1	11.951935000	6.360546000	0.067703000
6	11.507759000	6.333238000	2.193777000
1	12.558438000	6.293686000	2.495421000
6	9.815541000	6.430640000	0.442736000
1	9.543087000	6.464961000	-0.615286000
1	5.356209000	3.233457000	-0.583409000
1	7.390039000	3.086138000	-0.468797000
1	6.414024000	4.360482000	0.741599000
1	6.252853000	2.286871000	0.985798000
1	4.465083000	8.930560000	1.513381000
1	5.490957000	8.597058000	3.213058000
1	5.392810000	7.159085000	1.691823000
1	6.507416000	8.845393000	1.466490000

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PBE0-D2/(dppm)Cu(BH$_4$) E= -3314.18172578 Ha

29	-1.606718000	0.783497000	1.916359000
15	1.507600000	-0.811123000	1.295115000
15	-1.285981000	-0.291347000	0.064910000
6	0.191771000	-1.429824000	0.077068000
1	0.604473000	-1.548611000	-0.942277000
1	-0.165819000	-2.416193000	0.426093000
5	-1.911795000	1.933190000	3.642205000
1	-2.204461000	2.334019000	2.448420000
1	-1.563551000	0.685292000	3.645858000
1	-0.964865000	2.583518000	4.034285000
1	-2.923814000	2.013299000	4.298703000
6	1.637542000	0.960985000	0.778371000
6	1.154532000	1.941217000	1.678588000
6	2.119256000	1.367391000	-0.489530000
1	1.128710000	3.300341000	1.306511000
6	2.104805000	2.723127000	-0.853195000
1	1.603186000	3.690094000	0.042347000
1	0.801266000	1.649476000	2.673716000
1	2.502675000	0.616476000	-1.186221000
1	0.734054000	4.039263000	2.009145000
1	2.464293000	3.025263000	-1.841011000
1	1.583542000	4.744637000	-0.248725000
6	3.016174000	-1.521348000	0.495545000
6	4.258780000	-0.850870000	0.625184000
6	2.991127000	-2.777027000	-0.158591000
6	5.435351000	-1.414610000	0.104527000
6	4.171454000	-3.340493000	-0.677602000
6	5.396418000	-2.661194000	-0.549641000
1	4.295451000	0.123869000	1.120923000
1	2.047429000	-3.321198000	-0.263982000
1	6.383487000	-0.878360000	0.206962000
1	4.131559000	-4.310088000	-1.183153000
1	6.313243000	-3.098926000	-0.954590000
6	-2.650097000	-1.415000000	-0.444097000
6	-3.232890000	-1.396212000	-1.730459000
6	-3.134160000	-2.326945000	0.526098000
6	-4.276762000	-2.286541000	-2.044035000
6	-4.169725000	-3.219418000	0.204550000
6	-4.742923000	-3.200654000	-1.082034000
1	-2.876937000	-0.684196000	-2.479598000
1	-2.708242000	-2.324413000	1.535876000
1	-4.726237000	-2.262621000	-3.040953000
1	-4.537588000	-3.918912000	0.960404000
1	-5.555300000	-3.889901000	-1.328948000
6	-0.995974000	0.824614000	-1.357244000
6	-1.294594000	2.195763000	-1.197909000
6	-0.478557000	0.365091000	-2.591570000
6	-1.074014000	3.095526000	-2.255757000
6	-0.258971000	1.266314000	-3.646416000
6	-0.554970000	2.633568000	-3.478180000
1	-1.673315000	2.553221000	-0.234550000
1	-0.248148000	-0.695946000	-2.729515000
1	-1.296757000	4.157104000	-2.118403000
1	0.142785000	0.904254000	-4.597186000
1	-0.379132000	3.334795000	-4.299077000

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PBE0-D2/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6628.45069679 Ha

29	-2.761928000	6.565931000	-3.512181000
29	-0.783029000	5.958504000	-5.904405000
15	0.490218000	7.473798000	-4.865962000
15	-1.894749000	8.624279000	-3.505460000
15	-4.307835000	6.265702000	-5.095831000
15	-2.324097000	6.858815000	-7.237857000
5	-2.860818000	5.143795000	-1.867996000
1	-2.045421000	5.103557000	-2.861720000
1	-2.183087000	5.145813000	-0.858259000
1	-3.635855000	4.213385000	-1.966316000
1	-3.514141000	6.244347000	-1.897957000
5	0.102526000	3.973850000	-5.999443000
1	-0.349922000	2.997994000	-6.566735000
1	1.138569000	3.786878000	-5.392857000
1	0.287976000	4.882590000	-6.882450000
1	-0.792204000	4.367612000	-5.163646000
6	-0.445878000	9.057954000	-4.604427000
1	-0.807742000	9.385400000	-5.596124000
1	0.153092000	9.861535000	-4.137467000
6	-3.980708000	7.377181000	-6.547581000
1	-4.750127000	7.325279000	-7.339447000
1	-3.915523000	8.407438000	-6.153043000
6	1.981223000	7.976596000	-5.813221000
6	2.415577000	9.314166000	-5.946563000
1	1.860538000	10.124273000	-5.465122000
6	3.553339000	9.616320000	-6.717733000
1	3.881959000	10.655327000	-6.817216000
6	4.266065000	8.585821000	-7.359069000
1	5.149645000	8.822505000	-7.959017000
6	3.838151000	7.249733000	-7.228987000
1	4.386841000	6.446018000	-7.728168000
6	2.699406000	6.943201000	-6.464562000
1	2.348646000	5.908469000	-6.378633000
6	1.122725000	7.127588000	-3.179585000
6	1.876524000	8.087993000	-2.465772000
1	2.143356000	9.037774000	-2.940928000
6	2.279920000	7.824631000	-1.148432000
1	2.850119000	8.573910000	-0.592000000
6	1.936059000	6.600392000	-0.538683000
1	2.242819000	6.401859000	0.492608000
6	1.200268000	5.637056000	-1.250347000
1	0.924716000	4.689843000	-0.779938000
6	0.795817000	5.895711000	-2.573662000
1	0.219826000	5.155602000	-3.134656000
6	-1.326532000	9.220471000	-1.864123000
6	-0.983187000	10.574228000	-1.642391000
1	-1.106762000	11.307111000	-2.447409000
6	-0.505315000	10.979842000	-0.385708000
1	-0.243750000	12.028136000	-0.212561000
6	-0.371460000	10.036394000	0.653731000
1	0.001312000	10.354256000	1.632109000
6	-0.721034000	8.691907000	0.435839000
1	-0.615726000	7.956628000	1.238066000
6	-1.202600000	8.279444000	-0.820402000
1	-1.473112000	7.233626000	-0.998074000
6	-3.182684000	9.839726000	-4.008382000
6	-2.946309000	10.950513000	-4.850407000
1	-1.937688000	11.165557000	-5.212693000
6	-4.013486000	11.778097000	-5.248834000
1	-3.819714000	12.631041000	-5.906485000
6	-5.322536000	11.508430000	-4.807958000
1	-6.150040000	12.149206000	-5.126151000
6	-5.565865000	10.408735000	-3.961798000
1	-6.581347000	10.176866000	-3.630053000
6	-4.503391000	9.579202000	-3.566957000
1	-4.697923000	8.703739000	-2.938848000
6	-6.009185000	6.713783000	-4.564824000
6	-6.399516000	6.318857000	-3.261000000
1	-5.693401000	5.762482000	-2.634412000
6	-7.671820000	6.661519000	-2.772059000
1	-7.964667000	6.354068000	-1.764161000
6	-8.562183000	7.405727000	-3.571306000
1	-9.549513000	7.676273000	-3.185718000
6	-8.178569000	7.802243000	-4.866127000
1	-8.866677000	8.380842000	-5.489949000
6	-6.907766000	7.457558000	-5.361887000
1	-6.614455000	7.785498000	-6.362730000
6	-4.491287000	4.627415000	-5.899653000
6	-5.421859000	4.418809000	-6.944111000
1	-6.089565000	5.229856000	-7.253378000
6	-5.487725000	3.172907000	-7.585309000
1	-6.197771000	3.015991000	-8.402229000
6	-4.627252000	2.129684000	-7.185401000
1	-4.674165000	1.161747000	-7.693355000
6	-3.709205000	2.329779000	-6.139777000
1	-3.034250000	1.526964000	-5.832518000
6	-3.641023000	3.577624000	-5.491688000
1	-2.926342000	3.748085000	-4.682493000
6	-2.810542000	5.840702000	-8.686222000
6	-3.621625000	6.359191000	-9.721967000
1	-3.924732000	7.411898000	-9.702994000
6	-4.022237000	5.529443000	-10.781802000
1	-4.646759000	5.931750000	-11.585156000
6	-3.612873000	4.180525000	-10.812280000
1	-3.927602000	3.535012000	-11.637780000
6	-2.798157000	3.667023000	-9.787736000
1	-2.481219000	2.620830000	-9.806170000
6	-2.391206000	4.493782000	-8.724066000
1	-1.761034000	4.098308000	-7.920727000
6	-1.667931000	8.420402000	-7.961098000
6	-2.424639000	9.604001000	-8.122434000
1	-3.487246000	9.621502000	-7.865693000
6	-1.809194000	10.780257000	-8.591866000
1	-2.403039000	11.692415000	-8.705089000
6	-0.438154000	10.785232000	-8.909646000
1	0.037811000	11.703253000	-9.266401000
6	0.321229000	9.608187000	-8.760723000
1	1.391469000	9.605702000	-8.983447000
6	-0.289512000	8.434932000	-8.287925000
1	0.309323000	7.530841000	-8.135975000

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PBE0-D2/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6628.45053203 Ha

29	5.190521000	3.898987000	2.289741000
29	6.526351000	6.576017000	3.369613000
15	3.786170000	4.069464000	4.009156000
15	4.470914000	6.993400000	4.139917000
15	7.213770000	3.089504000	2.787339000
15	7.830516000	5.338335000	4.681500000
6	8.686551000	3.605430000	1.824704000
6	3.115400000	7.225988000	2.932577000
6	4.873510000	8.237787000	6.625003000
1	5.370910000	7.307387000	6.913830000
6	4.019996000	2.673007000	5.189359000
6	2.003013000	4.006375000	3.567954000
6	3.855113000	5.549870000	5.141961000
1	4.605313000	5.363755000	5.930934000
1	2.872206000	5.746385000	5.608531000
6	4.297751000	8.374112000	5.337855000
6	9.632335000	5.619577000	4.470656000
6	7.705388000	3.479435000	4.538569000
1	6.889163000	3.097019000	5.177431000
1	8.662697000	3.023430000	4.851603000
6	1.652509000	4.055360000	2.202200000
1	2.437438000	4.100770000	1.440593000
6	0.992357000	3.949515000	4.555297000
1	1.264476000	3.888569000	5.614669000
5	4.690676000	3.664708000	0.181872000
6	7.817261000	0.443601000	3.740153000
1	8.258825000	0.901176000	4.629639000
6	7.269470000	1.252203000	2.719350000
1	3.424486000	7.161581000	1.556390000
1	4.466059000	7.048900000	1.243945000
6	7.202540000	-1.564619000	2.499231000
1	7.174806000	-2.654954000	2.415370000
6	1.770089000	7.378537000	3.347193000
1	1.529741000	7.429740000	4.413753000
6	-0.360200000	3.952441000	4.178355000
1	-1.140949000	3.904991000	4.943490000
6	3.803416000	2.784830000	6.583723000
1	3.451947000	3.729904000	7.009175000
6	0.745707000	7.455192000	2.392021000
1	-0.294479000	7.554195000	2.714617000
6	4.823016000	9.302540000	7.539412000
1	5.274041000	9.180920000	8.528748000
6	6.695720000	4.872936000	7.274142000
1	6.225418000	3.970160000	6.873294000
6	3.682800000	9.596223000	4.980707000
1	3.239120000	9.708051000	3.987645000
6	2.391822000	7.235539000	0.602273000
1	2.636554000	7.166225000	-0.460665000
6	1.057216000	7.379478000	1.018742000
1	0.254922000	7.426754000	0.276322000
5	7.137490000	7.762475000	1.653861000
6	7.572439000	5.650271000	6.480093000
6	4.509675000	0.470145000	6.895824000
1	4.705744000	-0.378140000	7.557940000
6	8.510611000	4.485887000	0.736679000
1	7.505909000	4.827201000	0.476608000
6	4.048952000	1.688354000	7.431327000
1	3.880414000	1.785354000	8.508224000
6	0.295079000	4.058570000	1.830634000
1	0.028825000	4.106631000	0.771241000
6	4.205286000	10.516167000	7.180333000
1	4.170039000	11.346198000	7.891951000
6	6.682297000	0.637525000	1.585065000
1	6.232695000	1.263120000	0.806029000
6	4.478593000	1.442710000	4.661545000
1	4.667147000	1.355223000	3.586916000
6	8.161230000	6.807621000	7.048103000
1	8.843769000	7.414251000	6.445890000
6	6.655654000	-0.763277000	1.477312000
1	6.199770000	-1.228750000	0.598906000
6	4.721185000	0.347507000	5.509366000
1	5.094596000	-0.587685000	5.083804000
6	7.782100000	-0.959283000	3.629669000
1	8.207960000	-1.576989000	4.426317000
6	6.406371000	5.251543000	8.598988000
1	5.726898000	4.636651000	9.197105000
6	6.990104000	6.406817000	9.151069000
1	6.764107000	6.699277000	10.180393000
6	7.872460000	7.180352000	8.371394000
1	8.334283000	8.078026000	8.792110000
6	3.638533000	10.659999000	5.900303000
1	3.161531000	11.601897000	5.614067000
6	9.982506000	3.153644000	2.167331000
1	10.118006000	2.460548000	3.004031000
6	-0.709164000	4.009261000	2.813426000
1	-1.763486000	4.011554000	2.520692000
6	11.095244000	3.596994000	1.437966000
1	12.098299000	3.259937000	1.714104000
6	10.918804000	4.487990000	0.359022000
1	11.788758000	4.838697000	-0.204353000
6	9.630842000	4.927983000	0.007711000
1	9.490333000	5.624758000	-0.822472000
6	10.068546000	6.403529000	3.381941000
1	9.332426000	6.856523000	2.710280000
6	10.578991000	5.023761000	5.337616000
1	10.237821000	4.431693000	6.193743000
6	12.386566000	5.982842000	4.015583000
1	13.457242000	6.121230000	3.837460000
6	11.952423000	5.205249000	5.108779000
1	12.683777000	4.746322000	5.780934000
6	11.446685000	6.580322000	3.157347000
1	11.778802000	7.178085000	2.304446000
1	3.637096000	3.900397000	-0.378382000
1	5.585218000	3.287176000	-0.549556000
1	5.051412000	4.755470000	0.755831000
1	4.457927000	2.772106000	1.068256000
1	6.321971000	8.493386000	1.131900000
1	7.304010000	8.126207000	2.871298000
1	6.684199000	6.558243000	1.623060000
1	8.225248000	7.736441000	1.111145000

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PBE0-D3BJ/(dppm)Cu(BH$_4$) E= -3314.20502556 Ha

29	-1.473775000	0.414580000	2.173737000
15	1.512305000	-0.450653000	1.074544000
15	-1.335559000	-0.247749000	0.110817000
6	0.243458000	-1.207263000	-0.092564000
1	0.587768000	-1.283349000	-1.139557000
1	0.010278000	-2.224360000	0.273370000
5	-1.825374000	1.153286000	4.096442000
1	-1.417260000	1.882431000	3.108438000
1	-1.787764000	-0.106192000	3.795260000
1	-1.031621000	1.312070000	4.993743000
1	-2.975277000	1.452344000	4.335481000
6	1.883715000	1.114718000	0.161982000
6	1.284708000	2.305571000	0.632044000
6	2.673528000	1.157889000	-1.010526000
6	1.438912000	3.508638000	-0.078750000
6	2.841251000	2.364537000	-1.708096000
6	2.214997000	3.539102000	-1.249452000
1	0.684844000	2.281371000	1.548077000
1	3.160502000	0.246189000	-1.368516000
1	0.954892000	4.418575000	0.285266000
1	3.455380000	2.389138000	-2.613152000
1	2.337088000	4.475240000	-1.801267000
6	3.011364000	-1.454713000	0.680685000
6	4.265235000	-0.965754000	1.127612000
6	2.967542000	-2.714459000	0.041360000
6	5.437575000	-1.708917000	0.926998000
6	4.143989000	-3.461595000	-0.151801000
6	5.380973000	-2.961590000	0.286996000
1	4.317992000	0.006477000	1.627312000
1	2.016813000	-3.122414000	-0.311390000
1	6.396095000	-1.312624000	1.273419000
1	4.090609000	-4.434307000	-0.649114000
1	6.294204000	-3.543104000	0.135278000
6	-2.630295000	-1.408064000	-0.486722000
6	-2.981322000	-1.519943000	-1.850362000
6	-3.271657000	-2.230205000	0.468490000
6	-3.951115000	-2.453469000	-2.252175000
6	-4.236750000	-3.165825000	0.060518000
6	-4.576369000	-3.278859000	-1.299618000
1	-2.509089000	-0.867562000	-2.590055000
1	-3.019677000	-2.121039000	1.528814000
1	-4.222693000	-2.532597000	-3.308388000
1	-4.731137000	-3.795192000	0.805085000
1	-5.333812000	-4.001196000	-1.615636000
6	-1.318416000	1.105374000	-1.124008000
6	-2.104225000	2.244836000	-0.831022000
6	-0.583445000	1.066183000	-2.328261000
6	-2.158388000	3.320768000	-1.730137000
6	-0.629442000	2.151067000	-3.220126000
6	-1.417601000	3.276708000	-2.924898000
1	-2.653408000	2.288828000	0.115161000
1	0.046390000	0.205928000	-2.565979000
1	-2.766505000	4.197122000	-1.491318000
1	-0.040727000	2.119038000	-4.140690000
1	-1.447337000	4.120535000	-3.619436000

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PBE0-D3BJ/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6628.50645672 Ha

29	-2.774400000	6.541394000	-3.515371000
29	-0.773305000	5.944534000	-5.867440000
15	0.478111000	7.486542000	-4.819848000
15	-1.929817000	8.618097000	-3.451599000
15	-4.304861000	6.247874000	-5.132123000
15	-2.286307000	6.832851000	-7.259913000
5	-2.877112000	5.099626000	-1.877020000
1	-2.036727000	5.094407000	-2.849088000
1	-2.225398000	5.108357000	-0.851253000
1	-3.616855000	4.144178000	-2.001733000
1	-3.563365000	6.176653000	-1.913189000
5	0.099222000	3.945617000	-5.950016000
1	-0.331113000	2.976793000	-6.544352000
1	1.099183000	3.740178000	-5.291883000
1	0.338248000	4.857112000	-6.813578000
1	-0.836877000	4.339128000	-5.162328000
6	-0.483887000	9.051923000	-4.549034000
1	-0.852804000	9.367353000	-5.540683000
1	0.106200000	9.867744000	-4.095908000
6	-3.946047000	7.350531000	-6.582224000
1	-4.708844000	7.314318000	-7.379072000
1	-3.878526000	8.376493000	-6.180179000
6	1.938246000	8.024100000	-5.799482000
6	2.283605000	9.373999000	-6.026687000
1	1.676023000	10.178816000	-5.605402000
6	3.400336000	9.697315000	-6.817912000
1	3.657175000	10.746643000	-6.989611000
6	4.181799000	8.677175000	-7.387894000
1	5.049125000	8.930488000	-8.003814000
6	3.843882000	7.328725000	-7.164815000
1	4.445780000	6.530883000	-7.608051000
6	2.727539000	7.000741000	-6.379557000
1	2.450179000	5.953111000	-6.223816000
6	1.173611000	7.154614000	-3.152690000
6	1.941303000	8.125960000	-2.470048000
1	2.169804000	9.082617000	-2.950208000
6	2.415035000	7.865382000	-1.176639000
1	2.997253000	8.623955000	-0.646514000
6	2.131385000	6.631468000	-0.558409000
1	2.495809000	6.433279000	0.453526000
6	1.382107000	5.657338000	-1.238713000
1	1.154991000	4.700338000	-0.762842000
6	0.905021000	5.913751000	-2.536895000
1	0.318276000	5.161978000	-3.069415000
6	-1.358061000	9.205899000	-1.805586000
6	-1.021771000	10.559220000	-1.573809000
1	-1.152080000	11.299945000	-2.369719000
6	-0.540283000	10.958046000	-0.317499000
1	-0.283240000	12.006201000	-0.139485000
6	-0.396248000	10.010031000	0.714430000
1	-0.019653000	10.322912000	1.692440000
6	-0.742278000	8.667039000	0.489755000
1	-0.632759000	7.927405000	1.286920000
6	-1.227112000	8.261439000	-0.766263000
1	-1.496036000	7.216452000	-0.946009000
6	-3.208164000	9.855924000	-3.931735000
6	-2.969629000	10.962859000	-4.777658000
1	-1.967993000	11.156078000	-5.169301000
6	-4.024241000	11.821809000	-5.137693000
1	-3.827237000	12.671950000	-5.797377000
6	-5.323453000	11.590438000	-4.652775000
1	-6.141575000	12.257156000	-4.938664000
6	-5.569003000	10.495852000	-3.802925000
1	-6.578278000	10.295841000	-3.434995000
6	-4.520412000	9.633137000	-3.448016000
1	-4.719915000	8.763472000	-2.814286000
6	-6.004717000	6.729645000	-4.618850000
6	-6.456783000	6.246888000	-3.365986000
1	-5.798665000	5.612027000	-2.763946000
6	-7.730351000	6.598297000	-2.891366000
1	-8.068501000	6.221227000	-1.922477000
6	-8.564307000	7.438532000	-3.653401000
1	-9.553736000	7.715026000	-3.278815000
6	-8.120891000	7.922301000	-4.896625000
1	-8.764009000	8.576149000	-5.492824000
6	-6.847967000	7.569373000	-5.378618000
1	-6.512632000	7.966448000	-6.339761000
6	-4.541629000	4.606050000	-5.919457000
6	-5.465338000	4.420008000	-6.973558000
1	-6.088357000	5.253797000	-7.312103000
6	-5.586492000	3.165580000	-7.587591000
1	-6.291580000	3.028101000	-8.411797000
6	-4.791893000	2.087956000	-7.149090000
1	-4.882735000	1.112190000	-7.634640000
6	-3.884735000	2.264065000	-6.091047000
1	-3.263526000	1.432558000	-5.749734000
6	-3.759953000	3.520495000	-5.471108000
1	-3.055313000	3.666802000	-4.649417000
6	-2.762563000	5.816395000	-8.716194000
6	-3.543891000	6.347694000	-9.767866000
1	-3.829896000	7.404775000	-9.757791000
6	-3.938419000	5.525874000	-10.834691000
1	-4.541189000	5.939836000	-11.648121000
6	-3.551638000	4.171608000	-10.860252000
1	-3.861938000	3.532401000	-11.691717000
6	-2.763060000	3.645331000	-9.823485000
1	-2.459786000	2.595404000	-9.838824000
6	-2.363301000	4.463865000	-8.752108000
1	-1.752019000	4.055610000	-7.941947000
6	-1.628085000	8.382802000	-8.010403000
6	-2.345751000	9.596843000	-8.102186000
1	-3.382851000	9.656529000	-7.763801000
6	-1.725741000	10.751141000	-8.615781000
1	-2.290902000	11.685929000	-8.674770000
6	-0.389963000	10.704287000	-9.051334000
1	0.090274000	11.604410000	-9.444620000
6	0.329043000	9.496824000	-8.974196000
1	1.373402000	9.453347000	-9.292596000
6	-0.283298000	8.346367000	-8.454684000
1	0.289743000	7.418203000	-8.364073000

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PBE0-D3BJ/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6628.50644645 Ha

29	5.202176000	3.915868000	2.226976000
29	6.554724000	6.599401000	3.277025000
15	3.823207000	4.036437000	3.984988000
15	4.496957000	6.950827000	4.108279000
15	7.197047000	3.036449000	2.759714000

15	7.822607000	5.316497000	4.602656000
6	8.695957000	3.509754000	1.811614000
6	3.072335000	7.235895000	2.986191000
6	3.806561000	8.313428000	6.547088000
1	3.334308000	7.390856000	6.893586000
6	4.098561000	2.599726000	5.106777000
6	2.022449000	3.957657000	3.621012000
6	3.936611000	5.504078000	5.129231000
1	4.731882000	5.328849000	5.875257000
1	2.972655000	5.660248000	5.644132000
6	4.417712000	8.370251000	5.275812000
6	9.642065000	5.564224000	4.498828000
6	7.670774000	3.459975000	4.505818000
1	6.835710000	3.120723000	5.143814000
1	8.609164000	2.984543000	4.840187000
6	1.602962000	4.082886000	2.280184000
1	2.346668000	4.199569000	1.486518000
6	1.062792000	3.802427000	4.647314000
1	1.387223000	3.675609000	5.685589000
5	4.675132000	3.885215000	0.111129000
6	7.752384000	0.400606000	3.771232000
1	8.213745000	0.866588000	4.645424000
6	7.211631000	1.197190000	2.738367000
6	3.293384000	7.223429000	1.592707000
1	4.304040000	7.072173000	1.206997000
6	7.070479000	-1.621780000	2.594367000
1	7.014432000	-2.712526000	2.540047000
6	1.767052000	7.442801000	3.488752000
1	1.592402000	7.471139000	4.568686000
6	-0.305107000	3.789334000	4.334264000
1	-1.045642000	3.666289000	5.129781000
6	4.253496000	2.696242000	6.508154000
1	4.158805000	3.660725000	7.012834000
6	0.692813000	7.614800000	2.604536000
1	-0.317210000	7.762178000	2.996403000
6	3.817815000	9.437947000	7.391285000
1	3.343524000	9.381493000	8.375327000
6	7.232246000	4.706156000	7.365345000
1	7.344891000	3.644414000	7.132998000
6	5.044032000	9.571870000	4.862556000
1	5.537161000	9.613919000	3.885879000
6	2.211827000	7.394137000	0.709739000
1	2.389274000	7.366444000	-0.368040000
6	0.914766000	7.586161000	1.213482000
1	0.074125000	7.713402000	0.525552000
5	7.221142000	8.054079000	1.793134000
6	7.438673000	5.685459000	6.367534000
6	4.673208000	0.297164000	6.647576000
1	4.904749000	-0.590347000	7.242737000
6	8.565698000	4.461425000	0.778097000
1	7.579488000	4.866981000	0.541255000
6	4.543330000	1.549943000	7.271622000
1	4.665132000	1.639791000	8.355101000
6	0.230744000	4.069779000	1.973129000
1	-0.087530000	4.177492000	0.933112000
6	4.438173000	10.628498000	6.974138000
1	4.446663000	11.501897000	7.632104000
6	6.595087000	0.566004000	1.630296000
1	6.153538000	1.180359000	0.839020000
6	4.227783000	1.331452000	4.489005000
1	4.133240000	1.248973000	3.401848000
6	7.279093000	7.051968000	6.705117000
1	7.410786000	7.816507000	5.932963000
6	6.530099000	-0.834522000	1.559745000
1	6.051087000	-1.310744000	0.700041000
6	4.508879000	0.189489000	5.253894000
1	4.626435000	-0.776213000	4.756232000
6	7.680932000	-1.001682000	3.698499000
1	8.099765000	-1.608128000	4.506736000
6	6.863428000	5.087433000	8.668916000
1	6.701831000	4.319177000	9.430822000
6	6.704611000	6.446367000	8.991850000
1	6.411456000	6.738515000	10.003885000
6	6.918637000	7.429165000	8.007500000
1	6.778329000	8.487255000	8.241720000
6	5.049237000	10.692940000	5.707303000
1	5.535708000	11.615082000	5.378187000
6	9.967704000	2.973815000	2.118760000
1	10.071392000	2.222749000	2.908229000
6	-0.721902000	3.926550000	2.995715000
1	-1.788497000	3.916740000	2.753842000
6	11.099246000	3.402657000	1.410561000
1	12.083489000	2.995974000	1.658190000
6	10.967855000	4.364067000	0.388979000
1	11.853212000	4.701838000	-0.157065000
6	9.704165000	4.889269000	0.071614000
1	9.597195000	5.638465000	-0.716519000
6	10.155295000	6.354596000	3.449356000
1	9.470153000	6.825686000	2.738558000
6	10.526646000	4.962010000	5.422674000
1	10.130988000	4.372261000	6.256382000
6	12.422872000	5.912990000	4.227845000
1	13.503283000	6.045334000	4.121248000
6	11.912275000	5.134776000	5.285089000
1	12.593837000	4.669521000	6.002997000
6	11.545172000	6.522853000	3.316024000
1	11.935881000	7.127808000	2.493845000
1	3.612459000	4.214862000	-0.377829000
1	5.526647000	3.555649000	-0.689175000
1	5.108479000	4.898075000	0.773788000
1	4.451065000	2.914385000	0.913925000
1	6.407071000	8.861246000	1.391783000
1	7.380915000	8.202892000	3.052939000
1	6.778747000	6.871936000	1.553775000
1	8.316960000	8.129635000	1.273048000

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B3LYP/(dppm)Cu(BH$_4$) E= -3316.03659703 Ha

29	-1.665569000	0.468547000	2.216282000
15	1.592734000	-0.267292000	0.974078000
15	-1.388529000	-0.173625000	0.112713000
6	0.261574000	-0.999191000	-0.139646000
1	0.542852000	-1.035706000	-1.198248000
1	0.114018000	-2.032803000	0.199586000
5	-2.128504000	1.129760000	4.187356000
1	-1.769453000	1.899377000	3.229297000
1	-2.059456000	-0.097873000	3.827808000
1	-1.339565000	1.281268000	5.079120000
1	-3.276399000	1.374701000	4.449355000
6	2.109151000	1.235726000	0.022982000
6	1.741485000	2.491549000	0.543417000
6	2.848154000	1.189155000	-1.175457000
6	2.083340000	3.671000000	-0.129762000
6	3.195220000	2.367520000	-1.843242000
6	2.809056000	3.610568000	-1.323827000
1	1.192323000	2.544419000	1.479068000
1	3.167274000	0.231982000	-1.576734000
1	1.789416000	4.630826000	0.282747000
1	3.770501000	2.317828000	-2.762939000
1	3.080945000	4.524600000	-1.842515000
6	3.004762000	-1.422673000	0.664716000
6	4.141010000	-1.253585000	1.484963000
6	3.014332000	-2.466725000	-0.279574000
6	5.254622000	-2.086258000	1.351094000
6	4.126994000	-3.309032000	-0.405707000
6	5.250414000	-3.118987000	0.404646000
1	4.147130000	-0.468607000	2.235957000
1	2.157302000	-2.636530000	-0.922408000
6	6.119032000	-1.936719000	1.990302000
1	4.113181000	-4.110707000	-1.137850000
1	6.111446000	-3.772257000	0.305973000
6	-2.583144000	-1.449175000	-0.472578000
6	-2.858191000	-1.668271000	-1.835747000
6	-3.222618000	-2.252611000	0.491415000
6	-3.744723000	-2.677421000	-2.224398000
6	-4.106414000	-3.263985000	0.098799000
6	-4.367769000	-3.478302000	-1.258939000
1	-2.395429000	-1.043216000	-2.592044000
1	-3.035782000	-2.079164000	1.547310000
1	-3.952525000	-2.834604000	-3.278078000
1	-4.594655000	-3.873450000	0.852117000
1	-5.058193000	-4.258311000	-1.563432000
6	-1.514649000	1.183166000	-1.119391000
6	-2.406247000	2.235155000	-0.827262000
6	-0.805011000	1.215097000	-2.333961000
6	-2.593915000	3.282656000	-1.733714000
6	-0.988661000	2.268536000	-3.236452000
6	-1.885580000	3.300917000	-2.940701000
1	-2.944661000	2.237637000	0.115874000
1	-0.094699000	0.434100000	-2.579488000
1	-3.283457000	4.084889000	-1.492587000
1	-0.427072000	2.283951000	-4.164890000
1	-2.025028000	4.117704000	-3.641497000

110

B3LYP/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6632.10540056 Ha

29	-3.066931000	6.719456000	-3.407498000
29	-0.550939000	6.086066000	-6.128867000
15	0.482644000	7.627949000	-4.744871000
15	-1.975190000	8.730741000	-3.139853000
15	-4.348090000	6.296200000	-5.288539000
15	-2.231466000	6.724720000	-7.567504000
5	-3.453857000	5.244401000	-1.767522000
1	-2.459206000	5.240939000	-2.558572000
1	-3.021102000	5.263834000	-0.642081000
1	-4.150730000	4.292002000	-2.015543000
1	-4.118233000	6.306385000	-1.944797000
5	0.598772000	4.168691000	-6.260346000
1	0.378014000	3.222348000	-6.974625000
1	1.537469000	4.021282000	-5.517910000
1	0.803521000	5.172976000	-7.000802000
1	-0.446567000	4.371975000	-5.565996000
6	-0.515459000	9.125856000	-4.247363000
1	-0.913752000	9.545245000	-5.179100000
1	0.117015000	9.882054000	-3.767892000
6	-3.896307000	7.207710000	-6.854380000
1	-4.672042000	7.087859000	-7.619422000
1	-3.839830000	8.267897000	-6.580134000
6	1.918996000	8.374613000	-5.634585000
6	2.022542000	9.737318000	-5.967248000
1	1.247369000	10.437716000	-5.677774000
6	3.128981000	10.214582000	-6.682850000
1	3.193611000	11.270159000	-6.928810000
6	4.145287000	9.338388000	-7.074829000
1	5.002729000	9.709531000	-7.627274000
6	4.049914000	7.977713000	-6.753289000
1	4.831424000	7.289156000	-7.057900000
6	2.946445000	7.496938000	-6.044266000
1	2.874925000	6.438245000	-5.815378000
6	1.240566000	7.049003000	-3.172290000
6	2.122557000	7.863595000	-2.434123000
1	2.383581000	8.853224000	-2.796915000
6	2.678693000	7.400753000	-1.239988000
1	3.355880000	8.036051000	-0.677813000
6	2.364476000	6.117648000	-0.770324000
1	2.799124000	5.758768000	0.157392000
6	1.497543000	5.299491000	-1.500057000
1	1.254580000	4.303738000	-1.145260000
6	0.938055000	5.759800000	-2.699235000
1	0.282307000	5.113645000	-3.270773000
6	-1.334189000	9.109909000	-1.452336000
6	-0.876673000	10.395350000	-1.100260000
1	-0.911585000	11.205430000	-1.822593000
6	-0.399757000	10.649338000	0.187786000
1	-0.053599000	11.644627000	0.449220000
6	-0.378263000	9.623107000	1.142483000
1	-0.010751000	9.822129000	2.144417000
6	-0.838776000	8.347575000	0.804118000
1	-0.832683000	7.550220000	1.539817000
6	-1.317974000	8.088140000	-0.486698000
1	-1.684316000	7.097879000	-0.734272000
6	-3.116440000	10.147804000	-3.471981000
6	-2.722683000	11.363813000	-4.062820000
1	-1.694239000	11.518787000	-4.371102000
6	-3.649742000	12.393726000	-4.263373000
1	-3.328384000	13.324140000	-4.721316000
6	-4.982965000	12.226612000	-3.873654000
1	-5.700256000	13.026111000	-4.029610000
6	-5.387899000	11.022974000	-3.284387000
1	-6.421070000	10.880555000	-2.985354000
6	-4.464378000	9.991494000	-3.088097000
1	-4.791234000	9.058020000	-2.639757000
6	-6.082917000	6.852347000	-4.984066000
6	-6.768453000	6.251744000	-3.905556000
1	-6.275786000	5.489703000	-3.309744000
6	-8.072959000	6.639056000	-3.589922000
1	-8.585755000	6.164477000	-2.759537000
6	-8.713815000	7.637666000	-4.335426000
1	-9.726768000	7.938397000	-4.087130000
6	-8.040756000	8.246296000	-5.398851000
1	-8.528682000	9.022158000	-5.980956000
6	-6.734089000	7.856834000	-5.722592000
1	-6.234143000	8.345834000	-6.551079000
6	-4.572540000	4.552526000	-5.829349000
6	-5.557725000	4.191077000	-6.770154000
1	-6.220084000	4.945870000	-7.183278000
6	-5.701603000	2.859716000	-7.165424000
1	-6.462528000	2.591153000	-7.891428000
6	-4.867065000	1.872355000	-6.622879000
1	-4.981500000	0.837451000	-6.929885000
6	-3.893646000	2.220030000	-5.682111000
1	-3.248697000	1.460310000	-5.253984000
6	-3.746445000	3.554650000	-5.282361000
1	-3.003577000	3.815064000	-4.537681000
6	-2.679624000	5.521680000	-8.892150000
6	-3.524304000	5.869537000	-9.965219000
1	-3.921571000	6.876988000	-10.046063000
6	-3.839410000	4.931767000	-10.951268000
1	-4.487917000	5.211978000	-11.775697000
6	-3.311325000	3.635140000	-10.880460000
1	-3.554146000	2.907984000	-11.649126000
6	-2.466862000	3.284129000	-9.823565000
1	-2.049026000	2.284605000	-9.765035000
6	-2.148132000	4.221482000	-8.832198000
1	-1.483432000	3.941237000	-8.022531000
6	-1.764446000	8.239585000	-8.521100000
6	-2.678440000	9.224627000	-8.943057000
1	-3.732604000	9.137734000	-8.701547000
6	-2.244390000	10.333433000	-9.679171000
1	-2.963082000	11.083202000	-9.995332000
6	-0.891557000	10.474737000	-10.007558000
1	-0.556779000	11.334878000	-10.578619000
6	0.027892000	9.504111000	-9.593129000
1	1.080557000	9.608839000	-9.834074000
6	-0.403589000	8.398063000	-8.853863000
1	0.319897000	7.657631000	-8.526495000

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B3LYP/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6632.10482187 Ha

29	6.024019000	3.452991000	2.282444000
29	5.691499000	6.907449000	3.534030000
15	3.789613000	3.590492000	2.885146000
15	3.944257000	6.072524000	4.785109000
15	7.674957000	3.248611000	3.884159000
15	7.875618000	6.369464000	4.071420000
6	9.316609000	2.652331000	3.289659000
6	2.337454000	6.959954000	4.638016000
6	4.915905000	5.153381000	7.326515000
1	5.118127000	4.192675000	6.864199000
6	3.049908000	1.900040000	2.965088000
6	2.617710000	4.493957000	1.791698000
6	3.433050000	4.277759000	4.583780000
1	4.012288000	3.667485000	5.284375000
1	2.373536000	4.181464000	4.844885000
6	4.308853000	6.194786000	6.597979000
6	9.158623000	6.375945000	2.753735000
6	8.124992000	4.734008000	4.936674000
1	7.447929000	4.749179000	5.798637000
1	9.152567000	4.628352000	5.302935000
6	3.123531000	5.289865000	0.748755000
1	4.192550000	5.353039000	0.584785000
6	1.222970000	4.402195000	1.973168000
1	0.815335000	3.774464000	2.759906000
5	6.283241000	3.025210000	0.100871000
6	7.597114000	2.056899000	6.515561000
1	8.197140000	2.884978000	6.878036000
6	7.211966000	1.992507000	5.161767000
6	2.186359000	7.939395000	3.641363000
1	3.014517000	8.179531000	2.983358000
6	6.448405000	-0.031115000	6.977165000
1	6.154476000	-0.807701000	7.676019000
6	1.251856000	6.674060000	5.492094000
1	1.359164000	5.936991000	6.282792000
6	0.354076000	5.103941000	1.135340000
1	-0.718528000	5.027632000	1.283682000
6	2.480399000	1.337820000	4.122145000
1	2.428210000	1.904635000	5.044769000
6	0.038486000	7.349410000	5.344600000
1	-0.789872000	7.124088000	6.009237000
6	5.272177000	5.330427000	8.669111000
1	5.728520000	4.509298000	9.213464000
6	8.973165000	7.252713000	6.587107000
1	8.954190000	6.224219000	6.929351000
6	4.085281000	7.424857000	7.251325000
1	3.624432000	8.245570000	6.712370000
6	0.966225000	8.613912000	3.496774000
1	0.863039000	9.366922000	2.722590000
6	-0.106251000	8.320557000	4.343333000
1	-1.049588000	8.845775000	4.230182000
5	5.549831000	8.630131000	2.110595000
6	8.536900000	7.586038000	5.292283000
6	2.021562000	-0.727110000	2.931260000
1	1.624492000	-1.737212000	2.917851000
6	9.548487000	2.579654000	1.904905000
1	8.768166000	2.859698000	1.205861000
6	1.970683000	0.032470000	4.103821000
1	1.532376000	-0.384402000	5.005514000
6	2.248176000	5.993040000	-0.089285000
1	2.651592000	6.607040000	-0.887133000
6	5.037741000	6.552983000	9.306294000
1	5.314105000	6.689373000	10.346800000
6	6.434659000	0.896039000	4.736177000
6	6.117483000	0.833092000	3.699659000
6	3.104278000	1.120497000	1.788853000
1	3.557217000	1.528374000	0.890429000
6	8.562879000	8.940638000	4.895049000
1	8.208272000	9.221390000	3.908120000
6	6.059211000	-0.107949000	5.634826000
1	5.456538000	-0.939927000	5.286023000
6	2.589673000	-0.178325000	1.773839000
1	2.637420000	-0.761946000	0.860176000
6	7.216479000	1.053576000	7.415244000
1	7.524059000	1.118415000	8.454494000
6	9.434818000	8.245947000	7.460908000
1	9.767357000	7.971436000	8.457338000
6	9.468125000	9.582359000	7.052896000
1	9.827268000	10.350576000	7.730404000
6	9.029903000	9.926455000	5.767377000
1	9.045181000	10.962573000	5.445036000
6	4.445477000	7.600083000	8.590704000
1	4.262523000	8.554893000	9.073057000
6	10.338666000	2.263772000	4.178654000
1	10.170003000	2.285801000	5.251129000
6	0.866869000	5.902403000	0.103219000
1	0.190183000	6.446571000	-0.548232000
6	11.571100000	1.822426000	3.691589000
1	12.349954000	1.521670000	4.385625000
6	11.797330000	1.759982000	2.309569000
1	12.754527000	1.414028000	1.931890000
6	10.786567000	2.136651000	1.420930000
1	10.951809000	2.085913000	0.349868000
6	8.758791000	6.460474000	1.408303000
1	7.707140000	6.543005000	1.160788000
6	10.532359000	6.304743000	3.060389000
1	10.858666000	6.264442000	4.095265000
6	11.077036000	6.374941000	0.699517000
1	11.818518000	6.373503000	-0.093327000
6	11.484516000	6.302039000	2.039109000
1	12.540273000	6.245659000	2.285069000
6	9.717300000	6.455959000	0.386388000
1	9.395298000	6.517510000	-0.647510000
1	5.295980000	3.039500000	-0.591567000
1	7.306809000	2.806229000	-0.498356000
1	6.408115000	4.158189000	0.663217000
1	6.159486000	2.135148000	0.991184000
1	4.555884000	9.197959000	1.728912000
1	5.608660000	8.752510000	3.366947000
1	5.418133000	7.401426000	1.817276000
1	6.573444000	9.039437000	1.621372000

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B3LYP-D2/(dppm)Cu(BH$_4$) E= -3316.12855609 Ha

29	-1.653045000	0.803735000	1.928692000
15	1.516509000	-0.805382000	1.303838000
15	-1.301109000	-0.302046000	0.071527000
6	0.183269000	-1.422377000	0.107185000
1	0.588143000	-1.550552000	-0.904036000
1	-0.163372000	-2.401363000	0.460727000
5	-1.913480000	2.033388000	3.645628000
1	-2.224627000	2.386152000	2.456372000
1	-1.587767000	0.792878000	3.672652000
1	-0.950540000	2.673946000	3.984724000
1	-2.896080000	2.154089000	4.324335000
6	1.638650000	0.964147000	0.793857000
6	1.162887000	1.938267000	1.692714000
6	2.109708000	1.373195000	-0.470038000
6	1.133341000	3.291800000	1.325912000
6	2.094362000	2.722743000	-0.829045000
6	1.599949000	3.683380000	0.067061000
1	0.810182000	1.649776000	2.678303000
1	2.484456000	0.631422000	-1.167003000
1	0.741983000	4.022176000	2.025969000
1	2.445941000	3.024530000	-1.810403000
1	1.578310000	4.730469000	-0.219279000
6	3.007937000	-1.519963000	0.484481000
6	4.249268000	-0.857860000	0.589047000
6	2.966939000	-2.770148000	-0.164099000
6	5.409127000	-1.424431000	0.051276000
6	4.129745000	-3.337514000	-0.700956000
6	5.353784000	-2.666335000	-0.596615000
1	4.300204000	0.110150000	1.077261000
1	2.027241000	-3.306556000	-0.252223000
1	6.353885000	-0.896001000	0.135197000
1	4.077165000	-4.300542000	-1.199884000
1	6.254625000	-3.105124000	-1.013865000
6	-2.642811000	-1.435371000	-0.453366000
6	-3.221238000	-1.407790000	-1.734259000
6	-3.115786000	-2.363950000	0.496692000
6	-4.248581000	-2.302434000	-2.061884000
6	-4.134973000	-3.260430000	0.162991000
6	-4.703590000	-3.231022000	-1.118431000
1	-2.876257000	-0.689338000	-2.468867000
1	-2.695023000	-2.376112000	1.499054000
1	-4.691878000	-2.270889000	-3.052212000
1	-4.491718000	-3.970475000	0.902128000
1	-5.500229000	-3.921982000	-1.374994000
6	-0.999700000	0.814605000	-1.339288000
6	-1.296209000	2.179728000	-1.187133000
6	-0.469232000	0.357090000	-2.561254000
6	-1.063242000	3.074136000	-2.238575000
6	-0.236333000	1.251378000	-3.609598000
6	-0.532347000	2.612924000	-3.448000000
1	-1.682387000	2.542496000	-0.239710000
1	-0.239662000	-0.695361000	-2.695022000
1	-1.284839000	4.127849000	-2.105819000
1	0.174400000	0.890384000	-4.547245000
1	-0.347289000	3.307747000	-4.261201000

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B3LYP-D2/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6632.33611796 Ha

29	-2.839133000	6.605450000	-3.508229000
29	-0.754707000	5.955762000	-5.898283000
15	0.460020000	7.510726000	-4.784716000
15	-1.956387000	8.681174000	-3.408787000
15	-4.393418000	6.268973000	-5.117706000
15	-2.339624000	6.774007000	-7.281141000
5	-2.587382000	4.988649000	-2.028157000
1	-1.897083000	5.166361000	-3.080613000
1	-1.823309000	5.009155000	-1.094257000
1	-3.210770000	3.965472000	-2.154820000
1	-3.400285000	5.953038000	-1.898264000
5	0.291296000	4.013317000	-6.080278000
1	-0.047345000	3.032108000	-6.697804000
1	1.308892000	3.887788000	-5.443078000
1	0.431800000	4.956338000	-6.908738000
1	-0.658690000	4.293769000	-5.283288000
6	-0.502329000	9.073960000	-4.508643000
1	-0.843520000	9.407857000	-5.494446000
1	0.087549000	9.874399000	-4.046154000
6	-4.000767000	7.290997000	-6.619527000
1	-4.773644000	7.195817000	-7.391132000
1	-3.950185000	8.335035000	-6.295920000
6	1.917402000	8.063996000	-5.747775000
6	2.291575000	9.410798000	-5.898738000
1	1.717453000	10.196050000	-5.419299000
6	3.399737000	9.754005000	-6.684084000
1	3.679543000	10.797405000	-6.794960000
6	4.144377000	8.754376000	-7.323243000
1	5.001981000	9.021292000	-7.932985000
6	3.778136000	7.408893000	-7.175561000
1	4.349249000	6.630699000	-7.671580000
6	2.668955000	7.062018000	-6.396756000
1	2.369283000	6.021724000	-6.304112000
6	1.122305000	7.158989000	-3.120395000
6	1.839889000	8.134545000	-2.401429000
1	2.037388000	9.103573000	-2.850347000
6	2.295008000	7.860383000	-1.111635000
1	2.835633000	8.618718000	-0.554491000
6	2.039819000	6.607106000	-0.531988000
1	2.387454000	6.397571000	0.475060000
6	1.335665000	5.632074000	-1.245226000
1	1.124710000	4.667154000	-0.797906000
6	0.877683000	5.903643000	-2.541880000
1	0.320439000	5.155256000	-3.091949000
6	-1.342772000	9.162181000	-1.757075000
6	-0.924211000	10.478759000	-1.482174000
1	-1.015600000	11.245375000	-2.246670000
6	-0.406434000	10.802520000	-0.225629000
1	-0.086685000	11.818694000	-0.015522000
6	-0.304590000	9.812828000	0.764769000
1	0.099680000	10.064612000	1.740543000
6	-0.722697000	8.505338000	0.495592000
1	-0.638302000	7.735499000	1.254975000
6	-1.244448000	8.175717000	-0.762327000
1	-1.556935000	7.158483000	-0.972936000
6	-3.168983000	10.000187000	-3.817640000
6	-3.329128000	10.496039000	-5.126180000
1	-2.654215000	10.200196000	-5.921461000
6	-4.375727000	11.375239000	-5.432319000
1	-4.481653000	11.745015000	-6.447590000
6	-5.275516000	11.775534000	-4.436681000
1	-6.086741000	12.455861000	-4.675253000
6	-5.118432000	11.295749000	-3.128828000
1	-5.808377000	11.602584000	-2.349291000
6	-4.075516000	10.415853000	-2.821055000
1	-3.962624000	10.046789000	-1.807001000
6	-6.104138000	6.810863000	-4.757567000
6	-7.168220000	5.903663000	-4.608243000
1	-6.995758000	4.843533000	-4.757227000
6	-8.447008000	6.367015000	-4.272245000
1	-9.261326000	5.658369000	-4.157400000
6	-8.675311000	7.735756000	-4.083784000
1	-9.667478000	8.090992000	-3.823104000
6	-7.617266000	8.644614000	-4.226401000
1	-7.779955000	9.707039000	-4.074897000
6	-6.338794000	8.186955000	-4.556716000
1	-5.527141000	8.900490000	-4.646482000
6	-4.526394000	4.599084000	-5.832991000
6	-5.369830000	4.329620000	-6.930120000
1	-6.016206000	5.109479000	-7.321212000
6	-5.365911000	3.067008000	-7.524193000

1	-6.003094000	2.868663000	-8.379785000
6	-4.516086000	2.064702000	-7.030114000
1	-4.503589000	1.087139000	-7.502277000
6	-3.679229000	2.324731000	-5.940380000
1	-3.012938000	1.556620000	-5.563430000
6	-3.683491000	3.590078000	-5.336875000
1	-3.036035000	3.796942000	-4.492425000
6	-2.798555000	5.668560000	-8.664921000
6	-3.674479000	6.082634000	-9.686069000
1	-4.058781000	7.099004000	-9.692264000
6	-4.042176000	5.194355000	-10.699744000
1	-4.716520000	5.517890000	-11.486905000
6	-3.533398000	3.886027000	-10.701174000
1	-3.819542000	3.195626000	-11.488901000
6	-2.657180000	3.473952000	-9.691632000
1	-2.263874000	2.462868000	-9.686591000
6	-2.285757000	4.361193000	-8.672681000
1	-1.611785000	4.036260000	-7.887330000
6	-1.750254000	8.323520000	-8.073237000
6	-2.610649000	9.358061000	-8.490312000
1	-3.684767000	9.249218000	-8.379512000
6	-2.089233000	10.537451000	-9.036357000
1	-2.761632000	11.329017000	-9.353224000
6	-0.702900000	10.696910000	-9.172454000
1	-0.300946000	11.615381000	-9.588527000
6	0.161184000	9.671554000	-8.767097000
1	1.236177000	9.788544000	-8.851798000
6	-0.360404000	8.492237000	-8.222294000
1	0.313551000	7.709393000	-7.891720000

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B3LYP-D2/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6632.33626909 Ha

29	5.185731000	3.884083000	2.265385000
29	6.536824000	6.617801000	3.371638000
15	3.768332000	4.071996000	4.008631000
15	4.451762000	7.014784000	4.147908000
15	7.239758000	3.080748000	2.775733000
15	7.855992000	5.340506000	4.679583000
6	8.699354000	3.609951000	1.816616000
6	3.117351000	7.235762000	2.927057000
6	4.883243000	8.228651000	6.623581000
1	5.427048000	7.323351000	6.870413000
6	4.024436000	2.692308000	5.193990000
1	1.994779000	4.003999000	3.564818000
6	3.839691000	5.558209000	5.126197000
1	4.570469000	5.374697000	5.919857000
1	2.861960000	5.753121000	5.582819000
6	4.261186000	8.367546000	5.365501000
6	9.646998000	5.629140000	4.462749000
6	7.728049000	3.486918000	4.519922000
1	6.928668000	3.100219000	5.160981000
1	8.679676000	3.035688000	4.824690000
1	1.646707000	4.014248000	2.204463000
1	2.421334000	4.032048000	1.445480000
6	0.985121000	3.984440000	4.545613000
1	1.251838000	3.959529000	5.598663000
5	4.654663000	3.628423000	0.131459000
6	7.879086000	0.456521000	3.729363000
1	8.356603000	0.920282000	4.585425000
6	7.291352000	1.249561000	2.728273000
6	3.442307000	7.162024000	1.561701000
1	4.478208000	7.059177000	1.259591000
6	7.207709000	-1.557841000	2.552945000
1	7.173505000	-2.640873000	2.486769000
6	1.769905000	7.369618000	3.319136000
1	1.515207000	7.421369000	4.373222000
6	-0.360221000	3.984817000	4.169349000
1	-1.136463000	3.967619000	4.928409000
6	3.782247000	2.803866000	6.577180000
1	3.396926000	3.731834000	6.987370000
6	0.761576000	7.423710000	2.356124000
1	-0.275978000	7.508964000	2.662077000
6	4.816435000	9.261953000	7.562216000
5	5.302317000	9.138907000	8.525047000
6	6.678041000	4.875868000	7.235525000
6	6.196267000	3.999035000	6.817585000
6	3.582969000	9.561678000	5.062478000
1	3.104245000	9.677092000	4.096294000
6	2.425372000	7.211168000	0.598098000
1	2.682625000	7.133167000	-0.452432000
6	1.090434000	7.340425000	0.993858000
1	0.303475000	7.368097000	0.246430000
5	7.160188000	7.780653000	1.602479000
6	7.582957000	5.638748000	6.472253000
6	4.558395000	0.528052000	6.916111000
1	4.770588000	-0.302263000	7.582321000
6	8.519004000	4.508683000	0.753464000
1	7.523364000	4.855452000	0.504816000
6	4.048257000	1.727526000	7.432626000
1	3.858873000	1.824380000	8.497456000
6	0.295972000	4.015047000	1.831881000
1	0.034128000	4.033190000	0.779219000
6	4.135153000	10.448494000	7.255904000
1	4.086862000	11.252581000	7.983667000
6	6.655748000	0.622529000	1.636119000
1	6.175394000	1.229903000	0.873998000
6	4.531176000	1.480861000	4.686234000
1	4.737308000	1.387932000	3.625329000
6	8.179864000	6.771303000	7.062753000
1	8.881266000	7.367116000	6.488029000
6	6.620280000	-0.773277000	1.549984000
1	6.127692000	-1.246059000	0.706409000
6	4.797145000	0.404815000	5.541215000
1	5.206655000	-0.512050000	5.131317000
6	7.836421000	-0.941029000	3.642093000
1	8.292306000	-1.543923000	4.421803000
6	6.370024000	5.243131000	8.551894000
1	5.669253000	4.642068000	9.123253000
6	6.962901000	6.374373000	9.126457000
1	6.722673000	6.658474000	10.146001000
6	7.872488000	7.134502000	8.377875000
1	8.339489000	8.011266000	8.814900000
6	3.522077000	10.595970000	6.005447000
1	2.997552000	11.514470000	5.761130000
6	9.993448000	3.162247000	2.145783000
1	10.134051000	2.461681000	2.963755000
6	-0.705241000	4.002332000	2.808705000
1	-1.750973000	4.003813000	2.516261000
6	11.096921000	3.621454000	1.426374000
1	12.094641000	3.286531000	1.691031000
6	10.914312000	4.528615000	0.370170000
1	11.774576000	4.891863000	-0.183833000
6	9.630309000	4.969010000	0.033937000
1	9.485425000	5.678956000	-0.772700000
6	10.075736000	6.422299000	3.386283000
1	9.347572000	6.877704000	2.723905000
6	10.596321000	5.030047000	5.313807000
1	10.264400000	4.428849000	6.155888000
6	12.386881000	6.006823000	4.003987000
1	13.448135000	6.150488000	3.824851000
6	11.961480000	5.218172000	5.084620000
1	12.691284000	4.757096000	5.743255000
6	11.446226000	6.606393000	3.159866000
1	11.770227000	7.209620000	2.318672000
1	3.599531000	3.869233000	-0.404742000
1	5.526972000	3.248397000	-0.611256000
1	5.036984000	4.700526000	0.695853000
1	4.444034000	2.747241000	1.012896000
6	6.365046000	8.510348000	1.067208000
1	7.328189000	8.162256000	2.800102000
6	6.682619000	6.602927000	1.604924000
1	8.240965000	7.722680000	1.068273000

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B3LYP-D3BJ/(dppm)Cu(BH$_4$) E= -3316.19531257 Ha

29	-1.608194000	0.894451000	1.859937000
15	1.499402000	-0.794777000	1.281389000
15	-1.264091000	-0.270372000	0.027373000
6	0.200127000	-1.405073000	0.058191000
1	0.625326000	-1.525324000	-0.943333000
1	-0.151404000	-2.382352000	0.405633000
5	-1.986622000	2.140922000	3.545999000
1	-2.253564000	2.464572000	2.340741000
1	-1.570509000	0.932971000	3.606578000
1	-1.098400000	2.855390000	3.932831000
1	-3.011209000	2.194033000	4.167934000
6	1.676872000	0.954426000	0.729661000
6	1.226195000	1.959447000	1.605995000
6	2.165964000	1.324037000	-0.538105000
6	1.238212000	3.304487000	1.213118000
6	2.190640000	2.664885000	-0.923067000
6	1.720214000	3.656260000	-0.050217000
1	0.871594000	1.696258000	2.597306000
1	2.521747000	0.560743000	-1.221126000
1	0.867808000	4.061225000	1.895625000
1	2.555068000	2.936799000	-1.907940000
1	1.729294000	4.696816000	-0.357892000
6	3.008903000	-1.560156000	0.553637000
6	4.256443000	-0.925003000	0.719736000
6	2.977800000	-2.820258000	-0.072575000
6	5.430445000	-1.524449000	0.258514000
6	4.155205000	-3.420550000	-0.532432000
6	5.384499000	-2.774253000	-0.371331000
1	4.303356000	0.047370000	1.198514000
1	2.035883000	-3.342877000	-0.201961000
1	6.380117000	-1.015668000	0.388762000
1	4.109844000	-4.391323000	-1.015749000
1	6.296980000	-3.239025000	-0.729484000
6	-2.647699000	-1.356247000	-0.476775000
6	-2.485478000	-2.418011000	-1.385087000
6	-3.922976000	-1.099821000	0.057029000
6	-3.579430000	-3.204318000	-1.754320000
6	-5.017736000	-1.885643000	-0.316677000
6	-4.847169000	-2.937925000	-1.222137000
1	-1.507393000	-2.636040000	-1.800196000
1	-4.053012000	-0.290179000	0.768958000
1	-3.444342000	-4.023144000	-2.453184000
1	-5.996267000	-1.680326000	0.103521000
1	-5.695023000	-3.550975000	-1.508671000
6	-0.968433000	0.817296000	-1.416090000
6	-1.231983000	2.189935000	-1.280864000
6	-0.497830000	0.327971000	-2.647519000
6	-1.017701000	3.060062000	-2.354504000
6	-0.280773000	1.197960000	-3.717169000
6	-0.538540000	2.567496000	-3.571178000
1	-1.580242000	2.578335000	-0.329889000
1	-0.298751000	-0.730327000	-2.777189000
1	-1.214358000	4.119690000	-2.233266000
1	0.086314000	0.810940000	-4.661999000
1	-0.366884000	3.243003000	-4.402659000

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B3LYP-D3BJ/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6632.48392832 Ha

29	-2.786519000	6.507722000	-3.470875000
29	-0.741216000	5.891934000	-5.874906000
15	0.494699000	7.483607000	-4.823929000
15	-1.917737000	8.602682000	-3.441521000
15	-4.322529000	6.245888000	-5.122667000
15	-2.292801000	6.809061000	-7.249537000
5	-2.868584000	5.061930000	-1.793911000
1	-2.074250000	5.043848000	-2.784468000
1	-2.191651000	5.094290000	-0.796265000
1	-3.600079000	4.107894000	-1.878049000
1	-3.558164000	6.118441000	-1.834958000
5	0.127408000	3.858931000	-5.988310000
1	-0.344561000	2.918920000	-6.578361000
1	1.132311000	3.616701000	-5.369088000
1	0.368984000	4.768990000	-6.830042000
1	-0.754179000	4.270558000	-5.172596000
6	-0.499658000	9.022647000	-4.566417000
1	-0.880642000	9.314524000	-5.549198000
1	0.077112000	9.851173000	-4.144866000
6	-3.928829000	7.350024000	-6.554532000
1	-4.689292000	7.339401000	-7.340606000
1	-3.844662000	8.363510000	-6.152492000
6	1.933905000	8.049190000	-5.804138000
6	2.310281000	9.395394000	-5.941429000
1	1.749983000	10.176258000	-5.440621000
6	3.399195000	9.748059000	-6.745496000
1	3.677921000	10.792065000	-6.846861000
6	4.123890000	8.759420000	-7.419973000
1	4.967087000	9.034213000	-8.045206000
6	3.757824000	7.414021000	-7.285755000
1	4.314965000	6.642728000	-7.806835000
6	2.668663000	7.058859000	-6.485971000
1	2.372448000	6.018107000	-6.399224000
6	1.161786000	7.164879000	-3.153795000
6	1.923897000	8.127446000	-2.466124000
1	2.176640000	9.067079000	-2.946980000
6	2.355836000	7.879189000	-1.163902000
1	2.932033000	8.629154000	-0.632490000
6	2.033412000	6.666204000	-0.538336000
1	2.362464000	6.479101000	0.478659000
6	1.287645000	5.701339000	-1.220099000
1	1.027693000	4.765184000	-0.739567000
6	0.854832000	5.945683000	-2.528818000
1	0.271363000	5.201299000	-3.055971000
6	-1.330135000	9.208128000	-1.818938000
6	-0.975743000	10.554422000	-1.615942000
1	-1.097591000	11.274996000	-2.419390000
6	-0.483680000	10.971218000	-0.378109000
1	-0.212676000	12.010904000	-0.224727000
6	-0.346945000	10.047192000	0.667583000
1	0.037141000	10.372068000	1.629196000
6	-0.709490000	8.711672000	0.472874000
1	-0.603891000	7.992289000	1.277264000
6	-1.203789000	8.288971000	-0.766148000
1	-1.478211000	7.251733000	-0.917496000
6	-3.213318000	9.807912000	-3.928102000
6	-3.002997000	10.887149000	-4.804225000
1	-2.016661000	11.085798000	-5.205709000
6	-4.070765000	11.709487000	-5.183355000
1	-3.895643000	12.536095000	-5.864673000
6	-5.356704000	11.467907000	-4.688083000
1	-6.183607000	12.102211000	-4.989794000
6	-5.574284000	10.402946000	-3.805150000
1	-6.569504000	10.195701000	-3.428955000
6	-4.511425000	9.578950000	-3.430181000
1	-4.692099000	8.737125000	-2.770489000
6	-6.010790000	6.753194000	-4.626268000
6	-6.441785000	6.365458000	-3.341911000
1	-5.780603000	5.781780000	-2.709075000
6	-7.702099000	6.748445000	-2.875953000
1	-8.022387000	6.445873000	-1.884676000
6	-8.544421000	7.526393000	-3.680719000
1	-9.520676000	7.827329000	-3.314987000
6	-8.123125000	7.915040000	-4.956964000
1	-8.771058000	8.518931000	-5.584209000
6	-6.863469000	7.530024000	-5.427734000
1	-6.546778000	7.853914000	-6.412038000
6	-4.541835000	4.621811000	-5.929180000
6	-5.463654000	4.435987000	-6.976178000
1	-6.103373000	5.254558000	-7.290511000
6	-5.556359000	3.201119000	-7.616685000
1	-6.258270000	3.065702000	-8.432631000
6	-4.731533000	2.140607000	-7.214852000
1	-4.798410000	1.183092000	-7.721086000
6	-3.822768000	2.315197000	-6.168026000
1	-3.176669000	1.501741000	-5.858647000
6	-3.728615000	3.552942000	-5.520585000
1	-3.021004000	3.692608000	-4.712930000
6	-2.788799000	5.809524000	-8.698285000
6	-3.588162000	6.343427000	-9.725665000
1	-3.880509000	7.389143000	-9.698852000
6	-3.995715000	5.536219000	-10.788838000
1	-4.611640000	5.951908000	-11.579886000
6	-3.603358000	4.190990000	-10.836498000
1	-3.922804000	3.563773000	-11.662520000
6	-2.798517000	3.660819000	-9.824559000
1	-2.493785000	2.620656000	-9.855332000
6	-2.387316000	4.465933000	-8.756252000
1	-1.770196000	4.050225000	-7.968278000
6	-1.603768000	8.346923000	-7.977482000
6	-2.291376000	9.570688000	-8.051801000
1	-3.320810000	9.645870000	-7.723327000
6	-1.645978000	10.716670000	-8.532735000
1	-2.186625000	11.656752000	-8.578138000
6	-0.312770000	10.652058000	-8.951223000
1	0.187170000	11.543584000	-9.314981000
6	0.376567000	9.434295000	-8.894075000
1	1.415500000	9.376800000	-9.197855000
6	-0.263152000	8.292349000	-8.409486000
1	0.286454000	7.359707000	-8.336629000

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B3LYP-D3BJ/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6632.48388594 Ha

29	5.175473000	3.908004000	2.191443000
29	6.569948000	6.620846000	3.239167000
15	3.813602000	4.064483000	3.993125000
15	4.500505000	6.976294000	4.111100000
15	7.191049000	3.018608000	2.747611000
15	7.826461000	5.300056000	4.582649000
6	8.686720000	3.513035000	1.823649000
6	3.078249000	7.230745000	2.994281000
6	3.769270000	8.347439000	6.516199000
1	3.245235000	7.452937000	6.831645000
6	4.122432000	2.632058000	5.098019000
1	2.016681000	3.992087000	3.660988000
6	3.961026000	5.527139000	5.127762000
1	4.755636000	5.348051000	5.857802000
1	3.016972000	5.686453000	5.656896000
6	4.431874000	8.385203000	5.278527000
6	9.639191000	5.525434000	4.491176000
6	7.641829000	3.454017000	4.489344000
1	6.806043000	3.132312000	5.117277000
1	8.558125000	2.968193000	4.836869000
6	1.574858000	4.096922000	2.333063000
1	2.294012000	4.196670000	1.528538000
6	1.077424000	3.862687000	4.700338000
1	1.415142000	3.754307000	5.726945000
5	4.597329000	3.827754000	0.057674000
6	7.786923000	0.401595000	3.745019000
1	8.277633000	0.868360000	4.590985000
6	7.208225000	1.187905000	2.735188000
6	3.292099000	7.159554000	1.608603000
1	4.291615000	6.997602000	1.224776000
6	7.063723000	-1.618674000	2.616205000
1	7.006349000	-2.701338000	2.571869000
6	1.778430000	7.446862000	3.488320000
1	1.606698000	7.515027000	4.557748000
6	-0.288774000	3.854772000	4.414520000
1	-1.010263000	3.753150000	5.218903000
6	4.285797000	2.722731000	6.491232000
1	4.175111000	3.673519000	6.998362000
6	0.705711000	7.572420000	2.606586000
1	-0.296625000	7.726129000	2.991981000
6	3.796808000	9.456297000	7.368497000
1	3.284042000	9.413802000	8.324096000
6	7.179735000	4.720968000	7.323994000
1	7.294069000	3.666138000	7.105587000
6	5.125236000	9.554321000	4.906884000
1	5.655971000	9.583901000	3.960301000
6	2.211941000	7.282206000	0.726543000
1	2.384818000	7.205784000	-0.340787000
6	0.922164000	7.485673000	1.223757000
1	0.084545000	7.574140000	0.539550000
5	7.276328000	8.072549000	1.725347000
6	7.414307000	5.685993000	6.329184000
6	4.766633000	0.346528000	6.611041000
1	5.025429000	-0.531324000	7.193693000
6	8.560905000	4.474813000	0.808759000
1	7.583803000	4.869676000	0.559822000
6	4.609907000	1.585459000	7.241277000
1	4.738149000	1.670443000	8.315769000
6	0.204047000	4.088486000	2.051716000
1	-0.129145000	4.181144000	1.024027000
6	4.486231000	10.614204000	6.992738000
1	4.508294000	11.473311000	7.655207000
6	6.552625000	0.551870000	1.662135000
1	6.083737000	1.152989000	0.889188000
6	4.276386000	1.377250000	4.475117000
1	4.175172000	1.297218000	3.397955000
6	7.250535000	7.048392000	6.650964000
1	7.404869000	7.802362000	5.886250000
6	6.484952000	-0.842408000	1.603880000
1	5.976276000	-1.320773000	0.773686000
6	4.592996000	0.243533000	5.225208000
1	4.730535000	-0.707708000	4.724105000
6	7.714922000	-0.994033000	3.685292000
1	8.162467000	-1.590423000	4.473924000
6	6.776285000	5.110937000	8.607005000
1	6.592740000	4.355280000	9.364284000
6	6.610282000	6.465944000	8.912494000
1	6.289229000	6.764486000	9.904903000
6	6.854704000	7.435673000	7.932217000
1	6.710184000	8.487274000	8.151882000
6	5.148256000	10.661265000	5.759007000
1	5.686083000	11.555520000	5.462610000
6	9.957069000	2.999352000	2.144130000
1	10.060556000	2.248164000	2.920789000
6	-0.726554000	3.971143000	3.087650000
1	-1.789034000	3.966160000	2.866587000
6	11.087844000	3.456369000	1.468567000
1	12.067120000	3.068484000	1.728020000
6	10.958922000	4.427653000	0.465270000
1	11.841420000	4.789185000	-0.052448000
6	9.698987000	4.933256000	0.134662000
1	9.594069000	5.690567000	-0.633717000
6	10.166692000	6.319960000	3.461712000
1	9.501947000	6.805517000	2.756870000
6	10.508384000	4.900370000	5.404013000
1	10.105125000	4.304934000	6.218040000
6	12.413205000	5.839952000	4.239825000
1	13.487402000	5.958235000	4.140676000
6	11.889561000	5.055242000	5.277069000
1	12.556351000	4.572316000	5.984238000
6	11.552456000	6.472019000	3.338487000
1	11.951857000	7.078322000	2.533067000
1	3.535530000	4.165070000	-0.404214000
1	5.413940000	3.472281000	-0.753763000
1	5.067076000	4.827214000	0.684825000
1	4.388827000	2.886449000	0.874044000
1	6.500160000	8.896044000	1.311238000
1	7.425874000	8.232901000	2.969191000
1	6.789113000	6.920155000	1.509198000
1	8.367561000	8.098900000	1.212571000

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BP86/(dppm)Cu(BH$_4$) E= -3316.28679966 Ha

29	-1.495612000	0.526216000	1.990301000
15	1.463998000	-0.476592000	1.009444000
15	-1.370407000	-0.189751000	-0.071151000
6	0.255326000	-1.087700000	-0.310120000
1	0.648793000	-1.015955000	-1.340544000
1	0.041759000	-2.151387000	-0.094012000
5	-1.776030000	1.268071000	3.941172000
1	-1.540352000	2.006737000	2.904685000
1	-1.828482000	0.015626000	3.616376000
1	-0.848753000	1.403972000	4.707503000
1	-2.869528000	1.579009000	4.358241000
6	1.963690000	1.182024000	0.339832000
6	1.626111000	2.327076000	1.103038000
6	2.671198000	1.352232000	-0.876937000
6	1.976983000	3.615496000	0.652186000
6	3.023323000	2.638327000	-1.322602000
6	2.674628000	3.771934000	-0.559376000
1	1.090449000	2.205489000	2.050932000
1	2.962407000	0.474790000	-1.464375000
1	1.709354000	4.491041000	1.251693000
1	3.572558000	2.758450000	-2.262288000
1	2.952134000	4.772037000	-0.907611000
6	2.972999000	-1.489890000	0.623243000
6	4.217812000	-1.052751000	1.150500000
6	2.932602000	-2.730396000	-0.059857000
6	5.380963000	-1.823417000	0.986139000
6	4.099655000	-3.503920000	-0.219434000
6	5.326643000	-3.053653000	0.300187000
1	4.273691000	-0.100054000	1.687791000
1	1.992055000	-3.104686000	-0.475225000
1	6.330499000	-1.464769000	1.396302000
1	4.046225000	-4.458346000	-0.753498000
1	6.232089000	-3.655641000	0.175702000
6	-2.645056000	-1.445843000	-0.543986000
6	-3.048150000	-1.677839000	-1.880776000
6	-3.219561000	-2.219588000	0.495389000
6	-3.996848000	-2.675678000	-2.171465000
6	-4.164002000	-3.219896000	0.199292000
6	-4.552899000	-3.450119000	-1.134280000
1	-2.635931000	-1.069130000	-2.691080000
1	-2.933057000	-2.025029000	1.535425000
1	-4.305763000	-2.844039000	-3.208009000
1	-4.602827000	-3.808174000	1.010906000
1	-5.293551000	-4.222417000	-1.364008000
6	-1.467914000	1.099069000	-1.384435000
6	-2.208134000	2.270541000	-1.087750000
6	-0.879633000	0.966611000	-2.665799000
6	-2.367189000	3.279358000	-2.054848000
6	-1.035535000	1.980616000	-3.629563000
6	-1.781182000	3.136132000	-3.327099000
1	-2.646716000	2.391630000	-0.091104000
1	-0.292843000	0.078092000	-2.919016000
1	-2.939620000	4.179121000	-1.810196000
1	-0.571358000	1.868500000	-4.614427000
1	-1.898638000	3.924012000	-4.077496000

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BP86/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6632.61395301 Ha

29	-2.979129000	6.691885000	-3.448267000
29	-0.593262000	6.102240000	-6.100477000
15	0.474380000	7.592616000	-4.764310000
15	-1.980498000	8.705347000	-3.196160000
15	-4.308001000	6.292310000	-5.244331000
15	-2.224412000	6.759768000	-7.520408000
5	-3.266625000	5.193387000	-1.860377000
1	-2.281533000	5.240722000	-2.686759000
1	-2.795022000	5.196676000	-0.740606000
1	-3.949367000	4.222349000	-2.116607000
1	-3.968594000	6.256422000	-1.989089000
5	0.504467000	4.195362000	-6.216068000
1	0.274754000	3.233632000	-6.922350000
1	1.444724000	4.049830000	-5.461183000
1	0.718351000	5.195563000	-6.984770000
1	-0.559479000	4.417440000	-5.527156000
6	-0.497178000	9.117174000	-4.277263000
1	-0.880238000	9.548091000	-5.221464000
1	0.141172000	9.866044000	-3.771725000
6	-3.900004000	7.234344000	-6.810708000
1	-4.683685000	7.108443000	-7.581169000
1	-3.848497000	8.300263000	-6.518669000
6	1.936847000	8.308673000	-5.649889000
6	2.067577000	9.675526000	-5.991960000
1	1.291469000	10.394910000	-5.715421000
6	3.199945000	10.130953000	-6.697392000
1	3.287738000	11.192516000	-6.951169000
6	4.213207000	9.229014000	-7.069545000
1	5.092919000	9.584810000	-7.615142000
6	4.088690000	7.864009000	-6.739202000
1	4.869568000	7.154319000	-7.029603000
6	2.959974000	7.403872000	-6.039783000
1	2.862954000	6.339844000	-5.800090000
6	1.228800000	7.019242000	-3.178539000
6	2.124248000	7.839717000	-2.447797000
1	2.393398000	8.832052000	-2.825440000
6	2.685922000	7.377992000	-1.245562000
1	3.376678000	8.017527000	-0.686834000
6	2.362705000	6.092977000	-0.762610000
1	2.803022000	5.734769000	0.173476000
6	1.480982000	5.270492000	-1.486619000
1	1.229516000	4.271244000	-1.119711000
6	0.916208000	5.728166000	-2.693691000

1	0.246428000	5.081852000	-3.266499000
6	-1.383124000	9.136867000	-1.495840000
6	-0.966665000	10.449125000	-1.160526000
1	-1.008391000	11.248392000	-1.908539000
6	-0.527571000	10.743946000	0.141665000
1	-0.212333000	11.762046000	0.392611000
6	-0.504744000	9.732755000	1.124187000
1	-0.166790000	9.964669000	2.139378000
6	-0.924736000	8.430166000	0.799837000
1	-0.916639000	7.642630000	1.559324000
6	-1.365392000	8.128487000	-0.504323000
1	-1.703754000	7.115608000	-0.746605000
6	-3.135743000	10.110216000	-3.570013000
6	-2.738485000	11.329880000	-4.171310000
1	-1.697508000	11.488071000	-4.469836000
6	-3.675421000	12.357519000	-4.395221000
1	-3.351501000	13.293321000	-4.862244000
6	-5.020371000	12.184063000	-4.018139000
1	-5.746741000	12.984204000	-4.192016000
6	-5.427716000	10.976010000	-3.419107000
1	-6.472453000	10.827821000	-3.130446000
6	-4.495151000	9.946045000	-3.199878000
1	-4.821380000	9.004343000	-2.745361000
6	-6.045444000	6.832422000	-4.888510000
6	-6.705340000	6.204493000	-3.798651000
1	-6.185579000	5.432841000	-3.221153000
6	-8.015701000	6.574528000	-3.450865000
1	-8.511149000	6.078309000	-2.610561000
6	-8.686834000	7.581047000	-4.174942000
1	-9.707142000	7.867961000	-3.901463000
6	-8.037749000	8.216303000	-5.249203000
1	-8.550673000	8.999935000	-5.816511000
6	-6.725187000	7.845522000	-5.605306000
1	-6.239349000	8.354983000	-6.442512000
6	-4.558325000	4.552897000	-5.815424000
6	-5.582132000	4.218218000	-6.736623000
1	-6.252795000	4.995347000	-7.118595000
6	-5.756697000	2.886014000	-7.147174000
1	-6.549736000	2.635189000	-7.858848000
6	-4.915109000	1.874618000	-6.639574000
1	-5.054749000	0.836781000	-6.958731000
6	-3.903209000	2.198111000	-5.717762000
1	-3.251626000	1.417105000	-5.315357000
6	-3.724557000	3.532450000	-5.301945000
1	-2.953059000	3.780479000	-4.568561000
6	-2.673520000	5.576333000	-8.873880000
6	-3.505430000	5.954559000	-9.956875000
1	-3.892400000	6.977290000	-10.024792000
6	-3.816055000	5.030754000	-10.969654000
1	-4.455675000	5.333430000	-11.805206000
6	-3.295700000	3.721351000	-10.914088000
1	-3.535096000	3.004050000	-11.705797000
6	-2.463670000	3.342084000	-9.845367000
1	-2.051236000	2.329743000	-9.799241000
6	-2.149189000	4.263933000	-8.827100000
1	-1.490700000	3.967457000	-8.004222000
6	-1.756765000	8.287700000	-8.465364000
6	-2.675350000	9.288235000	-8.868106000
1	-3.735641000	9.205289000	-8.608624000
6	-2.239057000	10.406198000	-9.605486000
1	-2.961653000	11.171163000	-9.907853000
6	-0.881632000	10.538936000	-9.953935000
1	-0.544837000	11.407795000	-10.528147000
6	0.041435000	9.551699000	-9.557413000
1	1.100149000	9.650720000	-9.814700000
6	-0.390672000	8.437239000	-8.815774000
1	0.333966000	7.680404000	-8.496387000

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BP86/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6632.61357531 Ha

29	6.025795000	3.516160000	2.299384000
29	5.681489000	6.837492000	3.475765000
15	3.831441000	3.569908000	2.888120000
15	3.995700000	6.048095000	4.761431000
15	7.627948000	3.280599000	3.882673000
15	7.831673000	6.385109000	4.042286000
6	9.273413000	2.656446000	3.300524000
6	2.378779000	6.938762000	4.642962000
6	4.960543000	5.149327000	7.331589000
1	5.132219000	4.163035000	6.888035000
6	3.115066000	1.862425000	2.968344000
6	2.613505000	4.446578000	1.809145000
6	3.473131000	4.247900000	4.595799000
1	4.068803000	3.637244000	5.298378000
1	2.405120000	4.156312000	4.866182000
6	4.383413000	6.198331000	6.574168000
6	9.147529000	6.393858000	2.745737000
6	8.101967000	4.764091000	4.939418000
1	7.426063000	4.789677000	5.815256000
1	9.145072000	4.656372000	5.291113000
6	3.083803000	5.265145000	0.756289000
1	4.158195000	5.361886000	0.581674000
6	1.217775000	4.304198000	2.010662000
1	0.841475000	3.652171000	2.806366000
5	6.297386000	3.167526000	0.142463000
6	7.541574000	2.094207000	6.529392000
1	8.137754000	2.936487000	6.894628000
6	7.159263000	2.023759000	5.166364000
6	2.201520000	7.901625000	3.623280000
1	3.020506000	8.118113000	2.929295000
6	6.405606000	-0.018500000	6.988135000
1	6.115138000	-0.805160000	7.691477000
1	1.316506000	6.676505000	5.545558000
1	1.449579000	5.950215000	6.355091000
6	0.309825000	4.981791000	1.179755000
1	-0.766710000	4.866669000	1.341703000
6	2.551537000	1.289317000	4.133326000
1	2.499776000	1.859604000	5.065172000
6	0.096439000	7.363152000	5.423537000
1	-0.717051000	7.157594000	6.126958000
6	5.322840000	5.349156000	8.678280000
1	5.754898000	4.520139000	9.248189000
6	8.941030000	7.325312000	6.546820000
1	8.956239000	6.290000000	6.899228000
6	4.196370000	7.458495000	7.200360000
1	3.756156000	8.284938000	6.634351000
6	0.975125000	8.586556000	3.505387000
1	0.849093000	9.329531000	2.712193000
6	-0.075743000	8.319681000	4.401225000
1	-1.026002000	8.855507000	4.308995000
5	5.523693000	8.480619000	2.018229000
6	8.467638000	7.637166000	5.250509000
6	2.102940000	-0.787270000	2.928363000
1	1.710202000	-1.808853000	2.912518000
6	9.533215000	2.627710000	1.910821000
1	8.764836000	2.957603000	1.204195000
6	2.049195000	-0.027702000	4.111205000
1	1.612905000	-0.454789000	5.020213000
6	2.168849000	5.943114000	-0.073674000
1	2.544061000	6.576759000	-0.882398000
6	5.124712000	6.600881000	9.289321000
1	5.405949000	6.754395000	10.335723000
6	6.389037000	0.914538000	4.733604000
1	6.073933000	0.854171000	3.686201000
6	3.172860000	1.084227000	1.781393000
1	3.620968000	1.507310000	0.876128000
6	8.449113000	8.995018000	4.835083000
1	8.067054000	9.253553000	3.841839000
6	6.019329000	-0.099477000	5.636062000
1	5.421427000	-0.944404000	5.282158000
6	2.666382000	-0.226726000	1.763911000
1	2.715699000	-0.811715000	0.840271000
6	7.164904000	1.080554000	7.432675000
1	7.470530000	1.148422000	8.481935000
6	9.394299000	8.346025000	7.406440000
1	9.756602000	8.088988000	8.407220000
6	9.382822000	9.686828000	6.981900000
1	9.736864000	10.477956000	7.650440000
6	8.908268000	10.007833000	5.694051000
1	8.889999000	11.049359000	5.358353000
6	4.562965000	7.655260000	8.543365000
1	4.408002000	8.634772000	9.006363000
6	10.267362000	2.204007000	4.203555000
1	10.069177000	2.190453000	5.280901000
6	0.785308000	5.804044000	0.137319000
1	0.076286000	6.329700000	-0.510360000
6	11.504627000	1.741079000	3.723321000
1	12.264731000	1.388418000	4.428133000
6	11.760845000	1.721594000	2.336944000
1	12.723398000	1.356736000	1.964125000
6	10.775730000	2.163136000	1.435326000
1	10.965344000	2.144833000	0.357957000
6	8.773151000	6.447241000	1.383065000
1	7.715203000	6.497882000	1.113042000
6	10.522168000	6.363792000	3.089198000
1	10.825649000	6.351046000	4.141676000
6	11.123451000	6.414637000	0.726183000
1	11.889685000	6.422933000	-0.055673000
6	11.503475000	6.372167000	2.083663000
1	12.563216000	6.349285000	2.357287000
6	9.761182000	6.453601000	0.378342000
1	9.459379000	6.491630000	-0.672348000
1	5.302535000	3.177455000	-0.553867000
1	7.334819000	2.991865000	-0.465323000
1	6.400110000	4.300128000	0.744455000
1	6.203168000	2.238604000	1.018675000
1	4.519541000	9.021913000	1.598419000
1	5.551975000	8.646841000	3.285587000
1	5.409084000	7.226362000	1.760700000
1	6.558225000	8.889881000	1.530909000

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BP86-D2/(dppm)Cu(BH$_4$) E= -3316.38083161 Ha

29	-1.576581000	0.785544000	1.925590000
15	1.566691000	-0.873294000	1.308454000
15	-1.249535000	-0.318162000	0.097753000
6	0.199820000	-1.493109000	0.132485000
1	0.598631000	-1.663156000	-0.886129000
1	-0.179420000	-2.456874000	0.521852000
5	-1.909103000	1.943428000	3.644881000
1	-2.209790000	2.322557000	2.444492000
1	-1.547751000	0.698245000	3.655418000
1	-0.966294000	2.607580000	4.023939000
1	-2.920802000	2.018969000	4.302842000
6	1.636207000	0.916335000	0.834810000
6	1.116587000	1.854893000	1.762012000
6	2.083625000	1.371944000	-0.430602000
6	1.012732000	3.219064000	1.415699000
6	2.000791000	2.734364000	-0.765547000
6	1.454682000	3.657092000	0.153378000
1	0.798719000	1.529438000	2.759377000
1	2.489817000	0.651598000	-1.146952000
1	0.581331000	3.920011000	2.136290000
1	2.331519000	3.073010000	-1.752183000
1	1.374592000	4.714802000	-0.118202000
6	3.044984000	-1.532830000	0.410913000
6	4.277854000	-0.831431000	0.470702000
6	3.009223000	-2.783737000	-0.256029000
6	5.434709000	-1.361331000	-0.129593000
6	4.169452000	-3.313440000	-0.855020000
6	5.385008000	-2.603810000	-0.795333000
1	4.319940000	0.140604000	0.972896000
1	2.072771000	-3.349779000	-0.306946000
1	6.374833000	-0.801925000	-0.080786000
1	4.121726000	-4.279665000	-1.368399000
1	6.285910000	-3.014773000	-1.262021000
6	-2.648471000	-1.393576000	-0.414233000
6	-2.945933000	-1.686135000	-1.766296000
6	-3.442699000	-1.958184000	0.615002000
6	-4.015846000	-2.545566000	-2.081933000
6	-4.506068000	-2.823219000	0.294844000
6	-4.792528000	-3.118493000	-1.053786000
1	-2.355387000	-1.226775000	-2.565089000
1	-3.230498000	-1.703328000	1.660595000
1	-4.246337000	-2.763563000	-3.129777000
1	-5.116725000	-3.253532000	1.094688000
1	-5.625068000	-3.784010000	-1.303286000
6	-0.916281000	0.788625000	-1.323645000
6	-1.305951000	2.142517000	-1.198571000
6	-0.289462000	0.354343000	-2.516992000
6	-1.073452000	3.047884000	-2.251026000
6	-0.058025000	1.260819000	-3.567616000
6	-0.449140000	2.609516000	-3.434927000
1	-1.763123000	2.482918000	-0.262419000
1	0.028761000	-0.687509000	-2.626079000
1	-1.368212000	4.095757000	-2.139474000
1	0.429794000	0.917437000	-4.485565000
1	-0.263561000	3.315142000	-4.251135000

110

BP86-D2/[(dppm)Cu(BH$_4$)]$_2$ [1] E= -6632.85331963 Ha

29	-2.802710000	6.609878000	-3.546174000
29	-0.796406000	5.956182000	-5.864714000
15	0.423623000	7.498457000	-4.814049000
15	-1.967635000	8.663862000	-3.449561000
15	-4.378186000	6.288190000	-5.090914000
15	-2.342762000	6.780961000	-7.230858000
5	-2.531939000	5.000492000	-2.115539000
1	-1.840966000	5.196339000	-3.184971000
1	-1.745080000	4.999201000	-1.189266000
1	-3.171004000	3.979352000	-2.256599000
1	-3.340123000	5.983133000	-1.952240000
5	0.230905000	4.039369000	-6.021514000
1	-0.130064000	3.045647000	-6.623531000
1	1.272588000	3.920692000	-5.406203000
1	0.350873000	4.980617000	-6.878022000
1	-0.707043000	4.331827000	-5.194960000
6	-0.525804000	9.081060000	-4.566152000
1	-0.878693000	9.396270000	-5.565857000
1	0.066348000	9.896182000	-4.107179000
6	-4.004697000	7.333930000	-6.586891000
1	-4.783302000	7.242725000	-7.367420000
1	-3.940048000	8.384025000	-6.249717000
6	1.902675000	8.016323000	-5.773401000
6	2.288168000	9.364029000	-5.958989000
1	1.700601000	10.171379000	-5.511241000
6	3.420249000	9.676425000	-6.738522000
1	3.712507000	10.722706000	-6.878189000
6	4.173170000	8.645536000	-7.336382000
1	5.051054000	8.889810000	-7.943360000
6	3.792013000	7.299007000	-7.154266000
1	4.370947000	6.495786000	-7.620926000
6	2.659930000	6.981558000	-6.380960000
1	2.341222000	5.939253000	-6.258240000
6	1.085946000	7.178381000	-3.135786000
6	1.784877000	8.184574000	-2.425475000
1	1.961558000	9.160141000	-2.891694000
6	2.246704000	7.932399000	-1.124391000
1	2.772894000	8.715033000	-0.569243000
6	2.016036000	6.672356000	-0.528647000
1	2.369161000	6.480066000	0.489935000
6	1.330777000	5.667276000	-1.236480000
1	1.140034000	4.694304000	-0.775002000
6	0.866239000	5.915846000	-2.543999000
1	0.322085000	5.147422000	-3.099086000
6	-1.338638000	9.151775000	-1.797706000
6	-0.938473000	10.482638000	-1.524256000
1	-1.056786000	11.254536000	-2.293453000
6	-0.408603000	10.811704000	-0.264075000
1	-0.101421000	11.841105000	-0.051001000
6	-0.279850000	9.814023000	0.727062000
1	0.133417000	10.071477000	1.707996000
6	-0.680932000	8.491709000	0.456045000
1	-0.573890000	7.714600000	1.218321000
6	-1.212731000	8.155281000	-0.804671000
1	-1.511315000	7.124954000	-1.027210000
6	-3.201087000	9.979287000	-3.826882000
6	-3.373410000	10.509731000	-5.129429000
1	-2.685241000	10.244436000	-5.938591000
6	-4.443999000	11.382586000	-5.409829000
1	-4.562324000	11.781028000	-6.422812000
6	-5.351046000	11.743796000	-4.393647000
1	-6.181999000	12.421471000	-4.613336000
6	-5.178088000	11.231705000	-3.090426000
1	-5.874819000	11.510318000	-2.293609000
6	-4.113873000	10.355853000	-2.808015000
1	-3.986070000	9.956009000	-1.797113000
6	-6.097228000	6.807558000	-4.715149000
6	-7.150974000	5.878303000	-4.546963000
1	-6.958215000	4.811217000	-4.693580000
6	-8.440126000	6.328749000	-4.198558000
1	-9.250116000	5.603561000	-4.068804000
6	-8.687395000	7.704388000	-4.016770000
1	-9.690338000	8.050040000	-3.745754000
6	-7.638211000	8.633499000	-4.179024000
1	-7.815874000	9.703889000	-4.033347000
6	-6.348913000	8.190366000	-4.522277000
1	-5.539347000	8.919621000	-4.627997000
6	-4.503228000	4.626891000	-5.844811000
6	-5.386504000	4.366869000	-6.922889000
1	-6.074789000	5.147823000	-7.264241000
6	-5.368980000	3.114349000	-7.557752000
1	-6.038307000	2.919594000	-8.401256000
6	-4.465570000	2.118840000	-7.124544000
1	-4.443735000	1.148273000	-7.630967000
6	-3.585236000	2.373916000	-6.056675000
1	-2.872664000	1.611311000	-5.730045000
6	-3.602139000	3.627533000	-5.412102000
1	-2.918701000	3.841245000	-4.584873000
6	-2.821110000	5.684268000	-8.624377000
6	-3.703297000	6.115937000	-9.643562000
1	-4.081130000	7.145203000	-9.638842000
6	-4.081274000	5.230814000	-10.668339000
1	-4.761699000	5.566058000	-11.458289000
6	-3.576156000	3.912028000	-10.679918000
1	-3.870952000	3.222896000	-11.478382000
6	-2.694070000	3.484661000	-9.669329000
1	-2.304950000	2.462052000	-9.672162000
6	-2.311980000	4.367354000	-8.639178000
1	-1.633308000	4.037506000	-7.845142000
6	-1.718287000	8.319741000	-8.030156000
6	-2.557784000	9.389328000	-8.428967000
1	-3.642462000	9.310339000	-8.300016000
6	-2.002188000	10.561930000	-8.979033000
1	-2.658217000	11.384406000	-9.283196000
6	-0.605056000	10.677145000	-9.136395000
1	-0.176124000	11.592886000	-9.555878000
6	0.236931000	9.614690000	-8.749081000
1	1.323142000	9.698019000	-8.847859000
6	-0.317756000	8.442657000	-8.200777000
1	0.336410000	7.626706000	-7.877051000

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BP86-D2/[(dppm)Cu(BH$_4$)]$_2$ [2] E= -6632.85364032 Ha

29	5.202431000	3.946605000	2.258185000
29	6.524797000	6.576757000	3.367178000
15	3.813504000	4.114976000	3.981221000
15	4.491966000	7.020864000	4.164231000
15	7.189848000	3.099003000	2.803107000
15	7.807132000	5.344214000	4.685804000
6	8.687705000	3.608404000	1.879169000
6	3.131857000	7.221181000	2.957750000
6	4.884828000	8.239747000	6.656645000
1	5.408845000	7.316336000	6.923459000
6	4.069864000	2.678097000	5.104476000
6	2.027587000	4.069465000	3.556846000
6	3.900216000	5.558549000	5.158062000
1	4.665493000	5.358050000	5.929857000
1	2.923425000	5.743532000	5.644163000
6	4.294170000	8.384512000	5.375102000
6	9.609236000	5.604199000	4.460392000
6	7.650170000	3.485592000	4.567083000
1	6.812939000	3.122339000	5.192248000
1	8.594912000	3.015904000	4.901654000
6	1.667494000	4.083503000	2.191685000
1	2.448107000	4.105863000	1.423509000
1	1.024716000	4.051803000	4.555848000
1	1.308379000	4.024001000	5.614646000
5	4.688940000	3.675307000	0.157916000
6	7.804706000	0.451934000	3.742366000
1	8.274622000	0.910395000	4.617725000
6	7.228894000	1.262327000	2.736868000
6	3.435369000	7.086488000	1.583911000
1	4.475827000	6.956712000	1.272812000
6	7.130090000	-1.556492000	2.527589000
1	7.090006000	-2.647765000	2.447980000
6	1.786945000	7.386569000	3.373841000
1	1.554466000	7.482012000	4.439729000
6	-0.332665000	4.055204000	4.190248000
1	-1.108294000	4.038956000	4.963227000
6	3.942079000	2.751521000	6.513547000
1	3.635199000	3.690104000	6.987264000
6	0.756595000	7.417601000	2.420212000
1	-0.283318000	7.527171000	2.742628000
6	4.812140000	9.287805000	7.591174000
1	5.274561000	9.161087000	8.575409000
6	6.693370000	4.928034000	7.296869000
1	6.233172000	4.008673000	6.920534000
6	3.640123000	9.594921000	5.042862000
1	3.183630000	9.707871000	4.054730000
6	2.396614000	7.113102000	0.631332000
1	2.636114000	6.988374000	-0.428394000
6	1.062741000	7.278600000	1.048433000
1	0.255652000	7.288395000	0.308538000
5	7.113834000	7.655895000	1.578951000
6	7.558696000	5.694019000	6.477360000
6	4.619428000	0.411766000	6.709926000
1	4.840671000	-0.460787000	7.333037000
6	8.539254000	4.494493000	0.790400000
1	7.541043000	4.841370000	0.510844000
6	4.217454000	1.622506000	7.311469000
1	4.118363000	1.688109000	8.400177000
6	0.305062000	4.085641000	1.831281000
1	0.029334000	4.106501000	0.772631000
6	4.156076000	10.491357000	7.257587000
1	4.102871000	11.307983000	7.984975000
6	6.597652000	0.650635000	1.623170000
1	6.127176000	1.280639000	0.858548000
6	4.467135000	1.454957000	4.510025000
1	4.588224000	1.399158000	3.423147000
6	8.140411000	6.873431000	7.010282000
1	8.814462000	7.469184000	6.386508000
6	6.553537000	-0.752269000	1.521209000
1	6.062566000	-1.216914000	0.660281000
6	4.740355000	0.327920000	5.307493000
1	5.070903000	-0.599252000	4.830532000
6	7.755666000	-0.952444000	3.636889000
1	8.202365000	-1.572396000	4.421510000
6	6.403988000	5.342379000	8.613167000
1	5.732188000	4.739220000	9.232811000
6	6.979053000	6.520303000	9.130324000
1	6.752684000	6.840203000	10.152306000
6	7.853153000	7.280989000	8.325281000
1	8.307473000	8.195497000	8.719064000
6	3.573197000	10.642274000	5.983085000
1	3.066062000	11.575790000	5.718219000
6	9.974470000	3.152322000	2.255497000
1	10.084451000	2.458380000	3.096105000
6	-0.692477000	4.073080000	2.824739000
1	-1.750022000	4.075695000	2.540152000
6	11.107393000	3.595390000	1.555071000
1	12.103572000	3.257224000	1.856288000
6	10.958835000	4.492079000	0.473591000
1	11.844427000	4.843654000	-0.066167000
6	9.679889000	4.937727000	0.090828000
1	9.561848000	5.639913000	-0.739246000
6	10.044975000	6.379477000	3.363338000
1	9.307423000	6.827651000	2.688842000
6	10.555100000	5.005190000	5.327971000
1	10.210884000	4.418861000	6.187844000
6	12.365508000	5.949280000	3.993817000
1	13.432726000	6.081120000	3.811200000
6	11.930661000	5.177025000	5.093132000
1	12.662640000	4.715992000	5.764750000
6	11.424934000	6.548120000	3.133821000
1	11.758154000	7.138174000	2.275162000
1	3.631269000	3.926483000	-0.388219000
1	5.564072000	3.262227000	-0.577404000
1	5.087757000	4.764728000	0.707842000
1	4.452303000	2.804840000	1.064688000
1	6.304498000	8.381846000	1.041835000
1	7.320154000	8.072737000	2.774604000
1	6.621733000	6.466052000	1.626872000
1	8.187431000	7.564899000	1.016976000

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BP86-D3BJ/(dppm)Cu(BH4) E= -3316.44396646 Ha

29	-1.450435000	0.795663000	1.967046000
15	1.608433000	-0.873611000	1.238769000
15	-1.199996000	-0.284412000	0.106077000
6	0.238338000	-1.468215000	0.073476000
1	0.606848000	-1.613575000	-0.958034000
1	-0.137232000	-2.437664000	0.447015000
5	-1.816280000	1.884389000	3.728196000
1	-2.088227000	2.313345000	2.539759000
1	-1.410131000	0.655355000	3.694341000
1	-0.913573000	2.561326000	4.173786000
1	-2.850409000	1.894842000	4.353928000
6	1.704611000	0.908208000	0.750077000
6	1.214519000	1.859510000	1.679183000
6	2.145217000	1.350358000	-0.520884000
6	1.137255000	3.223477000	1.331239000
6	2.082940000	2.711570000	-0.859257000
6	1.569185000	3.647418000	0.062289000
1	0.912303000	1.538912000	2.682468000
1	2.530279000	0.623911000	-1.242001000
1	0.736380000	3.938463000	2.054793000
1	2.409572000	3.040659000	-1.849957000
1	1.507849000	4.705113000	-0.211561000
6	3.088172000	-1.557795000	0.369855000
6	4.336278000	-0.895442000	0.498584000
6	3.045046000	-2.785054000	-0.335646000
6	5.497486000	-1.434655000	-0.079532000
6	4.210632000	-3.324781000	-0.911345000
6	5.439264000	-2.650615000	-0.788832000
1	4.389984000	0.054071000	1.040257000
1	2.100719000	-3.329228000	-0.436326000
1	6.449172000	-0.903759000	0.021956000
1	4.156112000	-4.272430000	-1.456487000
1	6.344370000	-3.069390000	-1.238694000
6	-2.617541000	-1.357621000	-0.361299000
6	-3.141505000	-1.423853000	-1.671694000
6	-3.199144000	-2.145575000	0.662890000
6	-4.222666000	-2.278837000	-1.955422000
6	-4.272157000	-3.004474000	0.371851000
6	-4.785442000	-3.072642000	-0.938519000
1	-2.714073000	-0.801274000	-2.462403000
1	-2.818099000	-2.070054000	1.687791000
1	-4.627014000	-2.321035000	-2.971341000
1	-4.716410000	-3.607866000	1.168880000
1	-5.627489000	-3.734237000	-1.162494000
6	-0.932450000	0.827058000	-1.324655000
6	-1.309055000	2.181556000	-1.179162000
6	-0.369773000	0.392215000	-2.548006000
6	-1.120289000	3.087845000	-2.237287000
6	-0.179948000	1.300521000	-3.603113000
6	-0.552971000	2.650412000	-3.447972000
1	-1.722780000	2.521501000	-0.223948000
1	-0.072106000	-0.652718000	-2.679084000
1	-1.404281000	4.136204000	-2.109292000
1	0.260544000	0.956873000	-4.543903000
1	-0.398982000	3.357467000	-4.268682000

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BP86-D3BJ/[(dppm)Cu(BH4)]2 [1] E= -6633.00167138 Ha

29	-2.761633000	6.498215000	-3.514630000
29	-0.800601000	5.912683000	-5.792265000
15	0.421723000	7.524792000	-4.845478000
15	-1.952303000	8.571865000	-3.427812000
15	-4.296531000	6.321451000	-5.128276000
15	-2.261105000	6.796043000	-7.218521000
5	-2.865290000	5.060345000	-1.873704000
1	-2.045875000	5.045177000	-2.863064000

1	-2.192471000	5.077884000	-0.861881000
1	-3.610522000	4.107692000	-1.977298000
1	-3.547832000	6.138956000	-1.909341000
5	0.042491000	3.901178000	-5.837874000
1	-0.435905000	2.948179000	-6.420687000
1	1.040630000	3.661561000	-5.190536000
1	0.309883000	4.801374000	-6.704501000
1	-0.860056000	4.341049000	-5.036456000
6	-0.580824000	9.064917000	-4.583242000
1	-0.990461000	9.349521000	-5.568205000
1	-0.007344000	9.909737000	-4.163233000
6	-3.884237000	7.426112000	-6.563503000
1	-4.645866000	7.436453000	-7.362457000
1	-3.764564000	8.445032000	-6.155933000
6	1.838646000	8.091956000	-5.864992000
6	2.165145000	9.451185000	-6.068466000
1	1.572910000	10.239029000	-5.595360000
6	3.238391000	9.805503000	-6.906181000
1	3.479901000	10.861683000	-7.061386000
6	3.994467000	8.806482000	-7.547520000
1	4.828252000	9.083847000	-8.199850000
6	3.674554000	7.448041000	-7.348674000
1	4.257265000	6.667340000	-7.846726000
6	2.601425000	7.090020000	-6.515508000
1	2.334926000	6.036662000	-6.376892000
6	1.125139000	7.242790000	-3.175789000
6	1.857130000	8.246887000	-2.499436000
1	2.068159000	9.200432000	-2.994493000
6	2.309375000	8.023643000	-1.190597000
1	2.860626000	8.806953000	-0.662334000
6	2.038157000	6.795349000	-0.551963000
1	2.383473000	6.627824000	0.472907000
6	1.321113000	5.790430000	-1.225000000
1	1.100294000	4.840414000	-0.731290000
6	0.865281000	6.009902000	-2.538501000
1	0.298471000	5.238925000	-3.066144000
6	-1.333479000	9.155742000	-1.801680000
6	-0.953029000	10.501766000	-1.590501000
1	-1.072133000	11.237417000	-2.393923000
6	-0.439562000	10.898916000	-0.345231000
1	-0.145743000	11.940669000	-0.182195000
6	-0.311477000	9.956451000	0.696276000
1	0.090019000	10.267502000	1.665815000
6	-0.702623000	8.621218000	0.491153000
1	-0.603092000	7.886686000	1.295065000
6	-1.215648000	8.216597000	-0.755162000
1	-1.511783000	7.176810000	-0.923982000
6	-3.311329000	9.745627000	-3.825563000
6	-3.219643000	10.778595000	-4.786623000
1	-2.273079000	10.979250000	-5.295446000
6	-4.351969000	11.555056000	-5.103527000
1	-4.271265000	12.349978000	-5.851900000
6	-5.579417000	11.314258000	-4.458645000
1	-6.459334000	11.912297000	-4.713821000
6	-5.673638000	10.299246000	-3.486028000
1	-6.627062000	10.091329000	-2.993699000
6	-4.550138000	9.517952000	-3.174901000
1	-4.635285000	8.704393000	-2.447681000
6	-5.977489000	6.865745000	-4.626120000
6	-6.423968000	6.465657000	-3.342152000
1	-5.771164000	5.848926000	-2.715207000
6	-7.681876000	6.878464000	-2.871264000
1	-8.017528000	6.565789000	-1.877969000
6	-8.504553000	7.697224000	-3.671401000
1	-9.482193000	8.020961000	-3.301161000
6	-8.065174000	8.098775000	-4.946968000
1	-8.698129000	8.738312000	-5.570126000
6	-6.807585000	7.685290000	-5.422850000
1	-6.470711000	8.022263000	-6.406695000
6	-4.560909000	4.706311000	-5.955349000
6	-5.469533000	4.562754000	-7.030214000
1	-6.080157000	5.413133000	-7.350304000
6	-5.584394000	3.331134000	-7.691360000
1	-6.272657000	3.226548000	-8.535040000
6	-4.799340000	2.234556000	-7.277852000
1	-4.883899000	1.277530000	-7.801900000
6	-3.906179000	2.368932000	-6.200100000
1	-3.289532000	1.524455000	-5.881441000
6	-3.786173000	3.603664000	-5.534816000
1	-3.086639000	3.722475000	-4.704048000
6	-2.775679000	5.768467000	-8.649361000
6	-3.586458000	6.291444000	-9.683999000
1	-3.877971000	7.347629000	-9.670488000
6	-4.004337000	5.461052000	-10.736514000
1	-4.632174000	5.866401000	-11.536306000
6	-3.607625000	4.107904000	-10.765441000
1	-3.936005000	3.461619000	-11.585448000
6	-2.788346000	3.591380000	-9.745763000
1	-2.479996000	2.542391000	-9.763353000
6	-2.368913000	4.417687000	-8.686504000
1	-1.742282000	4.017125000	-7.883834000
6	-1.486447000	8.267687000	-8.003347000
6	-2.046741000	9.565661000	-8.001593000
1	-3.046233000	9.738593000	-7.592517000
6	-1.315388000	10.654154000	-8.518119000
1	-1.756769000	11.655942000	-8.507500000
6	-0.027462000	10.455254000	-9.048662000
1	0.542224000	11.303717000	-9.439061000
6	0.529719000	9.161218000	-9.070360000
1	1.537833000	9.000658000	-9.460902000
6	-0.190916000	8.076844000	-8.547760000
1	0.259934000	7.079293000	-8.529845000

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BP86-D3BJ/[(dppm)Cu(BH4)]2 [2] E= -6633.00147820 Ha

29	0.017573000	1.508997000	-1.207141000
29	-0.017595000	-1.509017000	-1.207139000
15	1.511250000	1.475592000	0.440319000
15	2.051617000	-1.306595000	-0.392087000
15	-2.051623000	1.306578000	-0.392048000
15	-1.511240000	-1.475611000	0.440351000
6	-3.365665000	0.596608000	-1.455162000
6	3.365634000	-0.596601000	-1.455218000
6	3.438574000	-2.979759000	1.484320000
1	3.566336000	-2.101403000	2.122359000
6	0.781115000	2.305961000	1.908451000
6	3.086509000	2.374377000	0.166139000
6	2.080530000	-0.174791000	1.081030000
1	1.347268000	-0.580134000	1.800752000
1	3.067192000	-0.088172000	1.568325000
6	2.768864000	-2.871881000	0.245382000
6	-3.086509000	-2.374394000	0.166207000
6	-2.080526000	0.174768000	1.081066000
1	-1.347271000	0.580110000	1.800795000
1	-3.067192000	0.088141000	1.568352000
6	3.349033000	2.884847000	-1.123226000
1	2.610201000	2.754407000	-1.919803000
6	4.039924000	2.536526000	1.198580000
1	3.825281000	2.163844000	2.206444000
5	0.223863000	2.472918000	-3.155547000
6	-3.438581000	2.979714000	1.484375000
1	-3.566386000	2.101336000	2.122374000
6	-2.768835000	2.871868000	0.245453000
6	3.030086000	-0.225331000	-2.775619000
1	2.020305000	-0.412344000	-3.149799000
6	-3.746010000	5.373043000	1.129276000
1	-4.123598000	6.341234000	1.472329000
6	4.673133000	-0.365491000	-0.966539000
1	4.938758000	-0.663211000	0.052963000
6	5.255429000	3.188788000	0.935834000
1	5.992670000	3.313520000	1.735254000
6	0.686938000	1.723219000	3.193050000
1	1.143241000	0.750202000	3.395395000
6	5.629286000	0.251548000	-1.786600000
1	6.634160000	0.447218000	-1.401453000
6	3.923755000	-4.225028000	1.923545000
1	4.436295000	-4.298206000	2.887857000
6	-0.686999000	-1.723252000	3.193101000
1	-1.143383000	-0.750275000	3.395453000
6	2.589364000	-4.031732000	-0.549181000
1	2.051409000	-3.954596000	-1.500036000
6	3.993462000	0.393147000	-3.594764000
1	3.722316000	0.694371000	-4.610079000
6	5.287363000	0.634689000	-3.100492000
1	6.032339000	1.125198000	-3.734615000
5	-0.223922000	-2.472921000	-3.155544000
6	-0.781074000	-2.305959000	1.908479000
6	-0.594923000	3.643693000	3.987579000
1	-1.138774000	4.154335000	4.787802000
6	-3.030156000	0.225391000	-2.775587000
1	-2.020392000	0.412433000	-3.149795000
6	-0.002915000	2.389657000	4.225516000
1	-0.072547000	1.927848000	5.215648000
6	4.567568000	3.540403000	-1.379233000
1	4.770646000	3.924175000	-2.382828000
6	3.746068000	-5.373068000	1.129140000
1	4.123670000	-6.341263000	1.472167000
6	-2.589289000	4.031743000	-0.549063000
1	-2.051313000	3.954628000	-1.499908000
6	0.186419000	3.573135000	1.681192000
1	0.232082000	4.017883000	0.682038000
6	-0.186266000	-3.573076000	1.681198000
1	-0.231852000	-4.017790000	0.682026000
6	-3.079074000	5.272886000	-0.108816000
1	-2.935514000	6.162502000	-0.729360000
6	-0.490804000	4.238157000	2.714263000
1	-0.966347000	5.201722000	2.514325000
6	-3.923744000	4.224977000	1.923634000
1	-4.436310000	4.298132000	2.887935000
6	0.002863000	-2.389673000	4.225573000
1	0.072416000	-1.927894000	5.215725000
6	0.594981000	-3.643654000	3.987616000
1	1.138835000	-4.154282000	4.787846000
6	0.490967000	-4.238081000	2.714274000
1	0.966597000	-5.201600000	2.514322000
6	3.079162000	-5.272880000	-0.108966000
1	2.935636000	-6.162477000	-0.729544000
6	-4.673150000	0.365480000	-0.966453000
1	-4.938745000	0.663172000	0.053065000
6	5.520605000	3.689503000	-0.355752000
1	6.468883000	4.196809000	-0.559117000
6	-5.629325000	-0.251535000	-1.786506000
1	-6.634188000	-0.447219000	-1.401340000
6	-5.287440000	-0.634625000	-3.100424000
1	-6.032435000	-1.125108000	-3.734545000
6	-3.993555000	-0.393059000	-3.594727000
1	-3.722442000	-0.694238000	-4.610064000
6	-3.349057000	-2.884887000	-1.123144000
1	-2.610232000	-2.754478000	-1.919732000
6	-4.039910000	-2.536515000	1.198665000
1	-3.825247000	-2.163821000	2.206521000
6	-5.520629000	-3.689502000	-0.355624000
1	-6.468915000	-4.196801000	-0.558966000
6	-5.255426000	-3.188767000	0.935950000
1	-5.992656000	-3.313476000	1.735383000
6	-4.567605000	-3.540432000	-1.379121000
1	-4.770700000	-3.924223000	-2.382705000
1	1.259145000	2.793701000	-3.704957000
1	-0.783312000	2.663193000	-3.805759000
1	0.317150000	1.217279000	-2.903894000
1	0.149416000	3.116661000	-2.055508000
1	0.783242000	-2.663186000	-3.805778000
1	-0.149446000	-3.116671000	-2.055510000
1	-0.317202000	-1.217281000	-2.903883000
1	-1.259212000	-2.793704000	-3.704936000