Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Superalkali Ligands as a Building block for Aromatic Trinuclear Cu(I)-NHC Complexes

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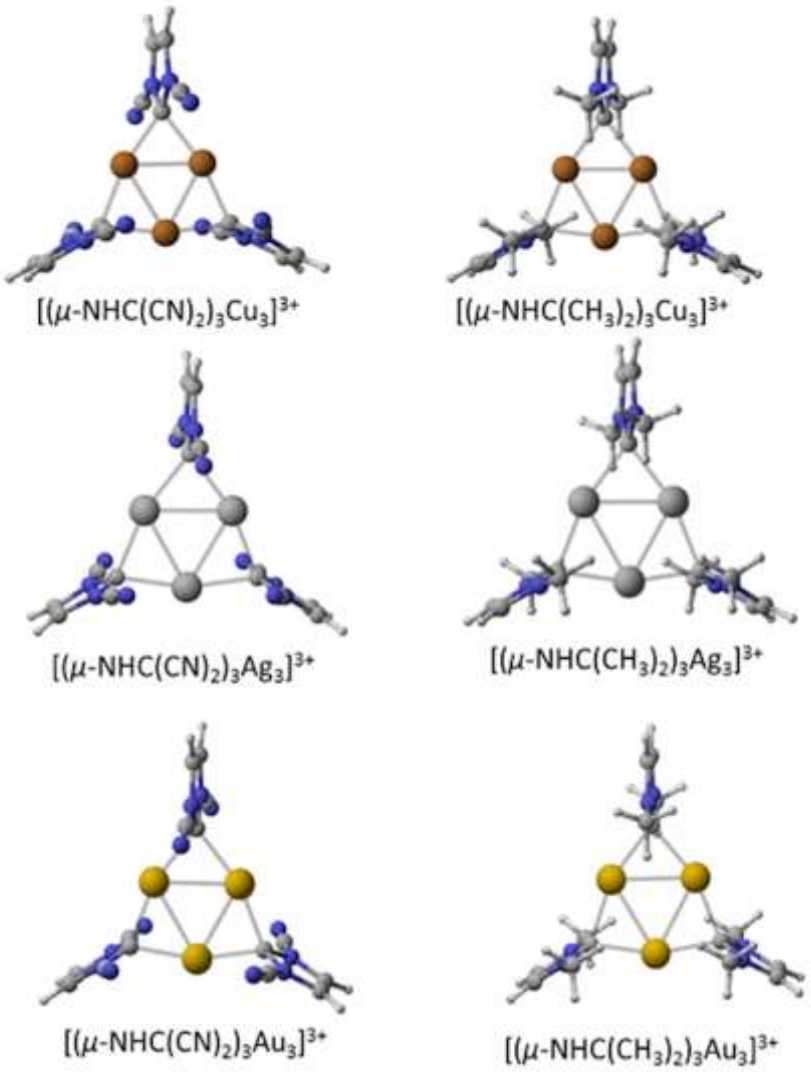


Figure S1: Optimized geometries of CN and CH_3 substituted imidazole with M_3 (M=Cu, Ag, Au).

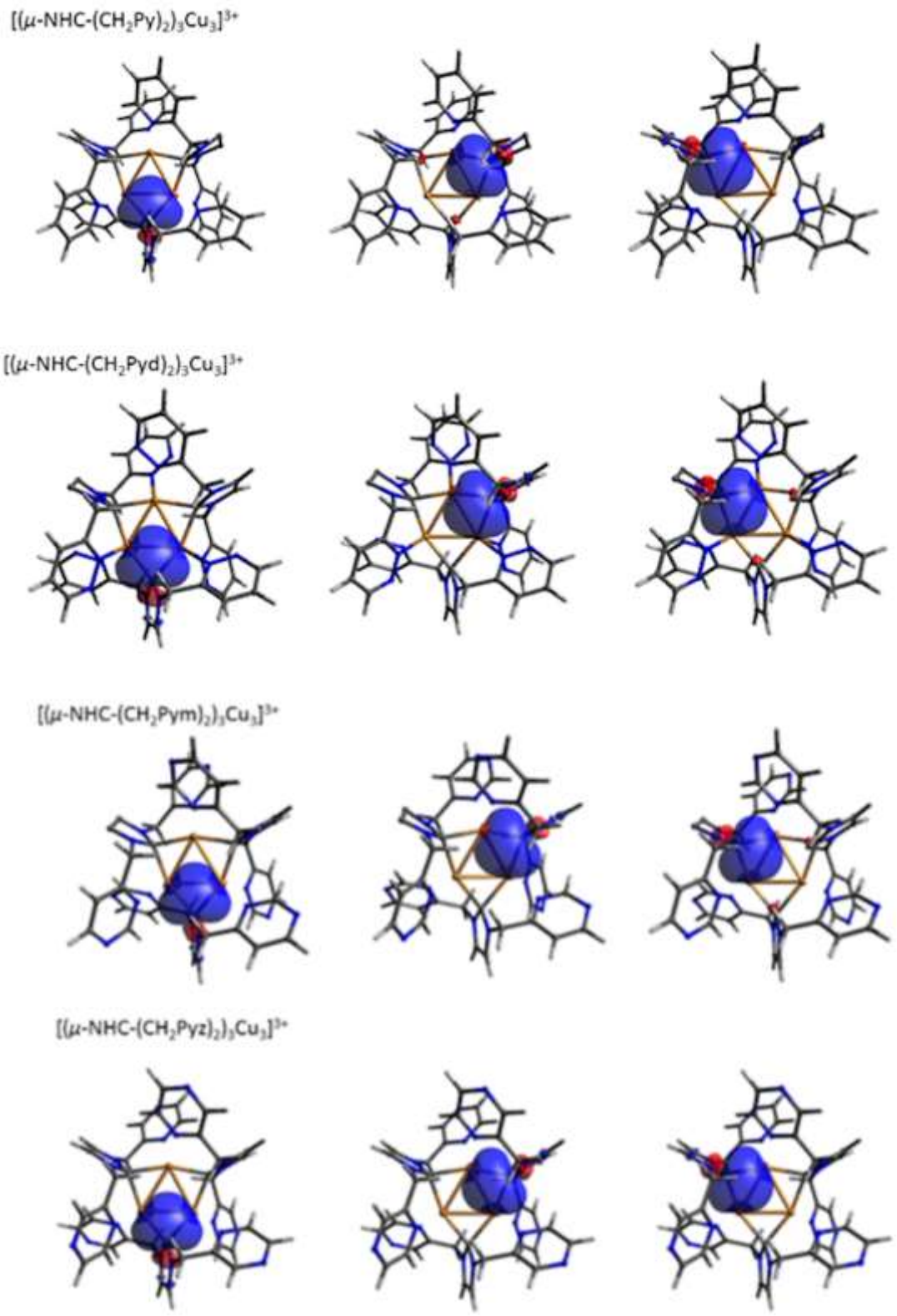


Figure S2: Hybridization of Cu_3-trinuclear complex with substituted NHC ligand.

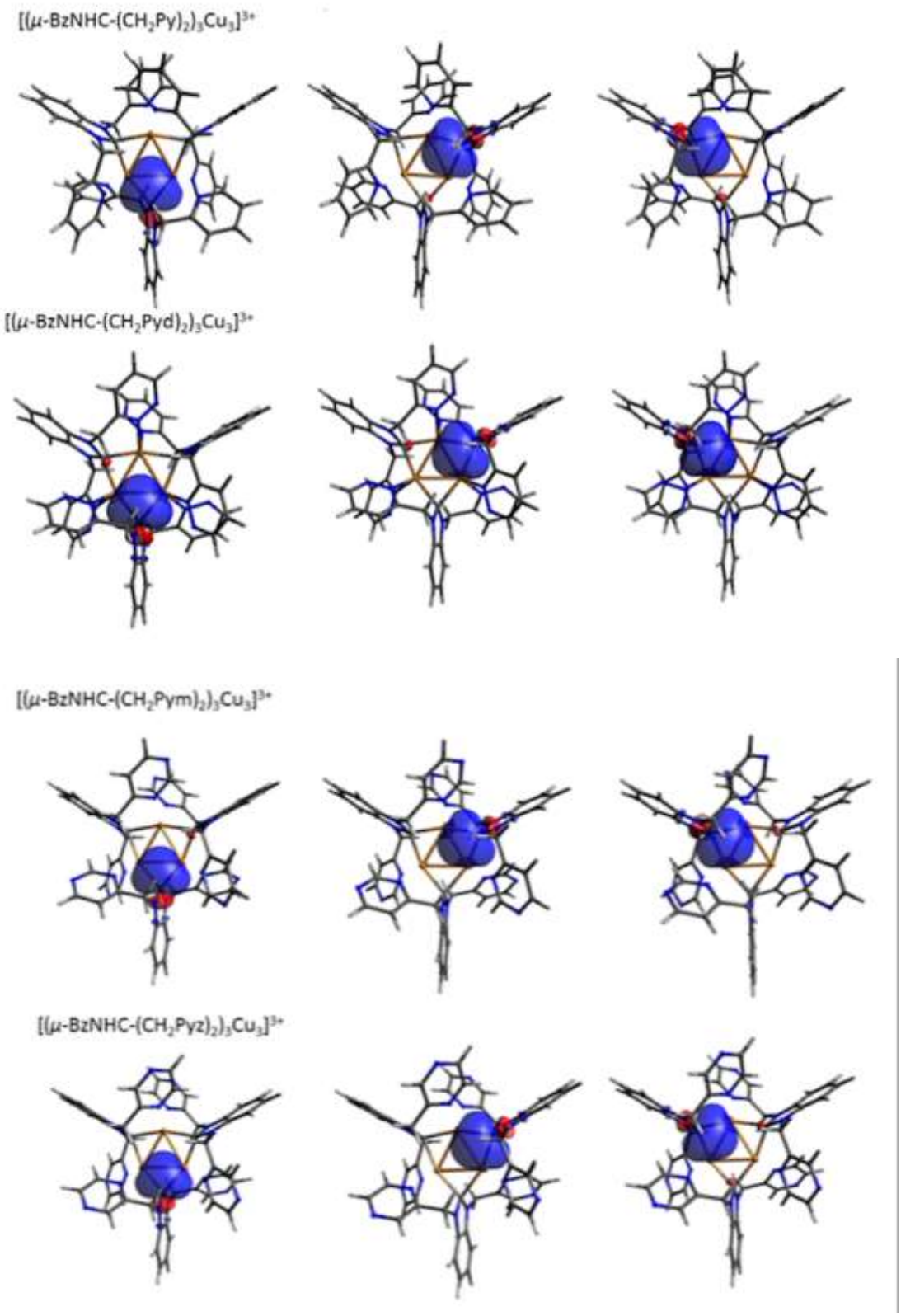
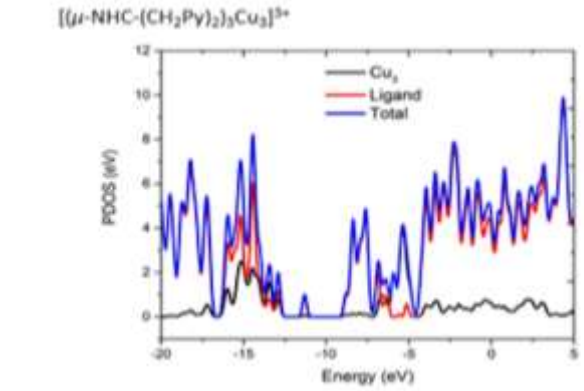
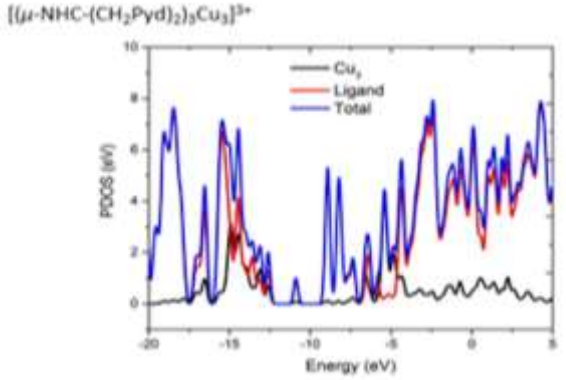


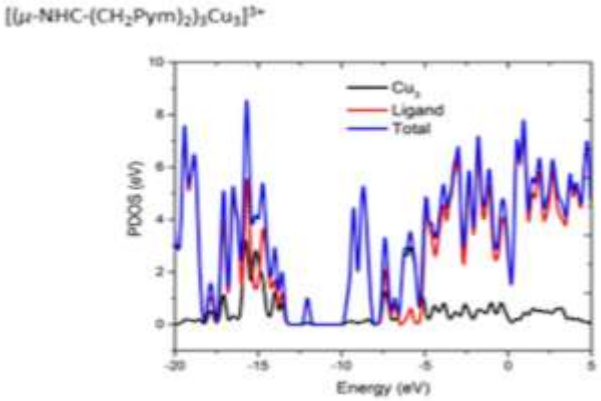
Figure S3: Hybridization of Cu_3-trinuclear complex with substituted Bz-NHC ligand.



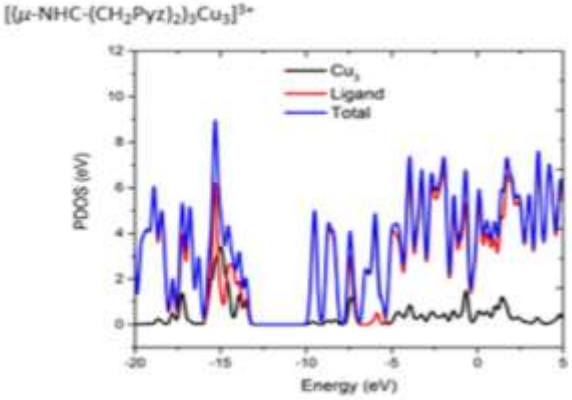
MOs	Cu_3	Ligand
L+5	1	99
L+4	3	97
L+3	6	94
L+2	3	97
L+1	11	89
LUMO	8	92
HOMO	47	53
H-1	34	66
H-2	69	31
H-3	66	34
H-4	63	37
H-5	53	47



MOs	Cu_3	Ligand
L+5	1	99
L+4	2	98
L+3	2	98
L+2	3	97
L+1	4	96
LUMO	9	91
HOMO	27	73
H-1	43	57
H-2	57	43
H-3	64	36
H-4	54	46
H-5	35	65

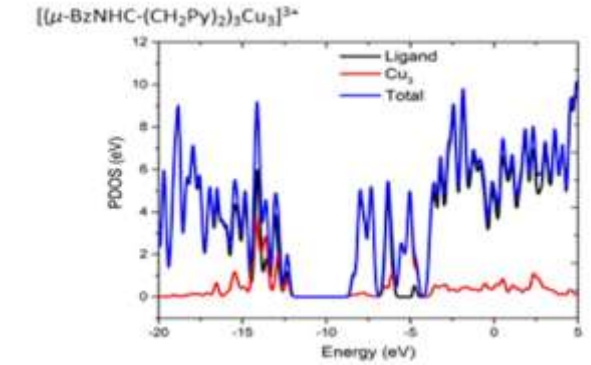


MOs	Cu_3	Ligand
L+5	1	99
L+4	2	98
L+3	4	96
L+2	3	97
L+1	10	90
LUMO	6	94
HOMO	45	55
H-1	35	65
H-2	46	54
H-3	49	51
H-4	34	66
H-5	15	85

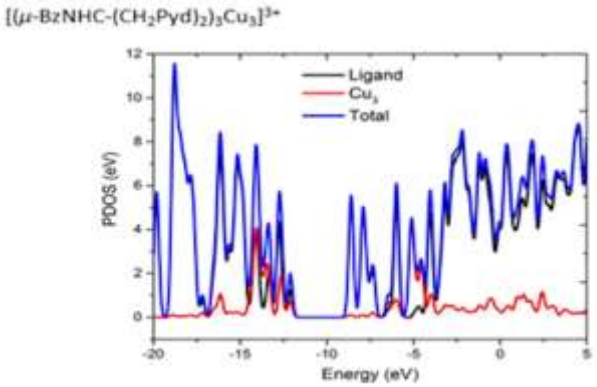


MOs	Cu_3	Ligand
L+5	2	98
L+4	2	98
L+3	1	99
L+2	1	99
L+1	3	97
LUMO	7	93
HOMO	47	53
H-1	47	53
H-2	43	57
H-3	43	57
H-4	43	57
H-5	15	85

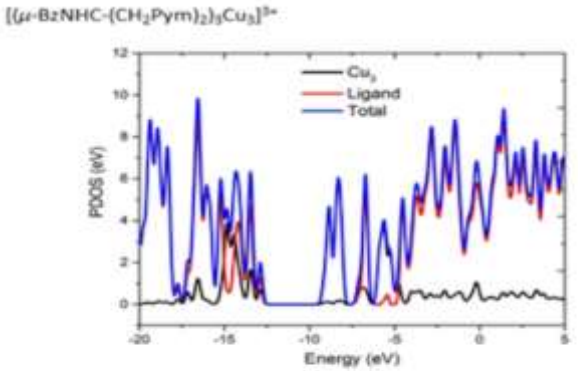
Figure S4. PDOS and % contribution of Cu_3-trinuclear complex with substituted NHC ligand.



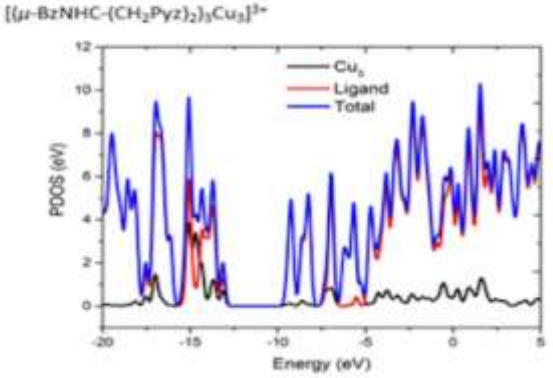
MOs	Ligand	Cu_3
L+5	98	2
L+4	98	2
L+3	96	4
L+2	95	5
L+1	97	3
LUMO	89	11
HOMO	59	41
H-1	59	41
H-2	35	65
H-3	31	69
H-4	31	69
H-5	99	1



MOs	Ligand	Cu_3
L+5	99	1
L+4	99	1
L+3	99	1
L+2	99	1
L+1	97	3
LUMO	96	4
HOMO	63	37
H-1	63	37
H-2	36	64
H-3	34	66
H-4	34	66
H-5	99	1



MOs	Cu_3	Ligand
L+5	1	99
L+4	1	99
L+3	3	97
L+2	3	97
L+1	3	97
LUMO	9	91
HOMO	35	65
H-1	35	65
H-2	35	65
H-3	34	66
H-4	33	67
H-5	21	79



MOs	Cu_3	Ligand
L+5	2	98
L+4	2	98
L+3	1	99
L+2	1	99
L+1	3	97
LUMO	8	92
HOMO	35	65
H-1	35	65
H-2	27	73
H-3	27	73
H-4	26	74
H-5	18	82

Figure S5. PDOS and % contribution of Cu_3-trinuclear complex with substituted Bz-NHC ligand.

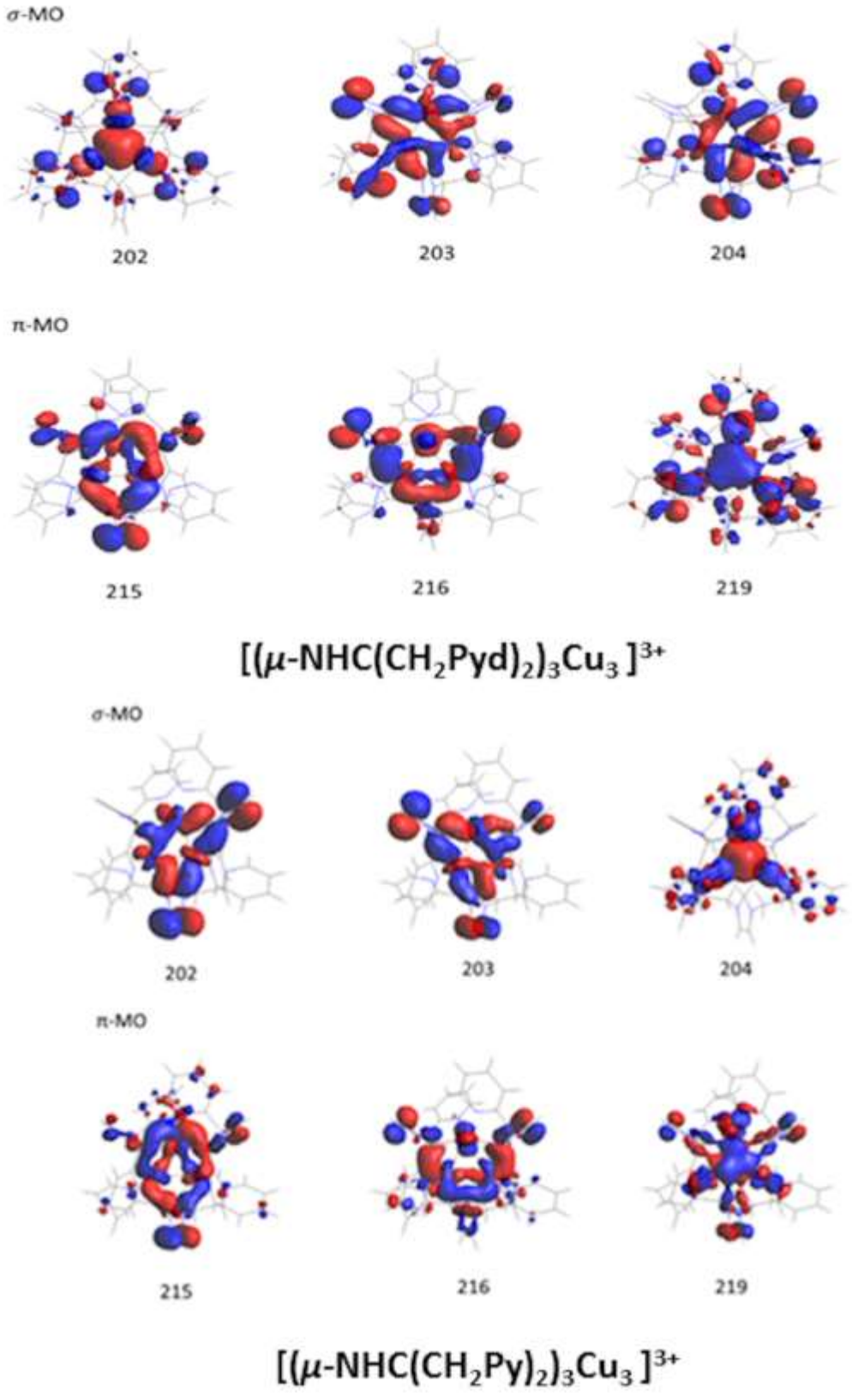


Figure S6: Canonical molecular orbital contribution towards the total NICS (0) with respect to to σ and π molecular orbital of $[(\mu\text{-NHC-R}_2)_3Cu_3]^{3+}$ (R= CH_2Pyd, CH_2Py) complexes.

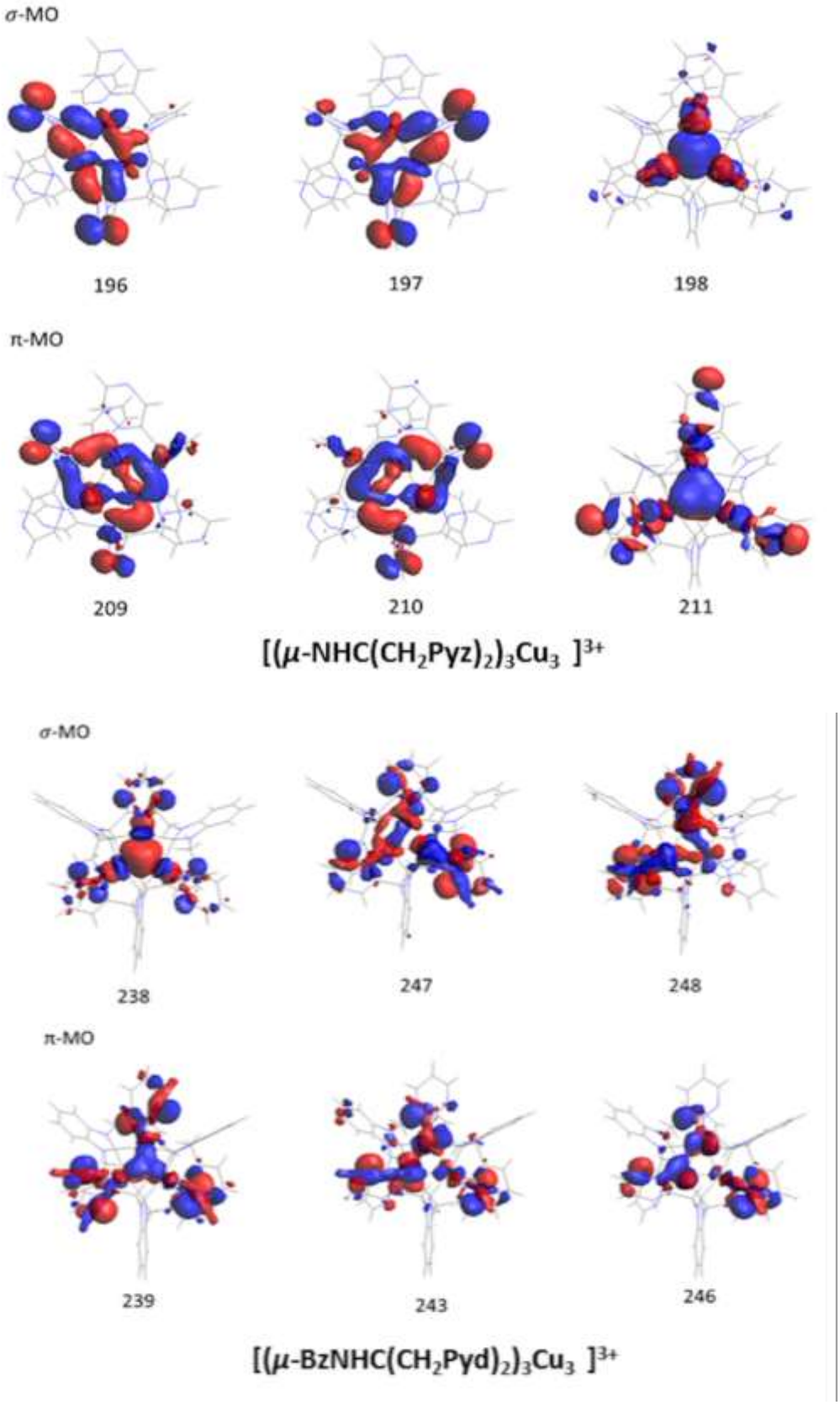


Figure S7: Canonical molecular orbital contribution towards the total NICS (0) with respect to to σ and π molecular orbital of $[(\mu\text{-NHC}(CH_2Pyz)_2)_3Cu_3]^{3+}$ and $[(\mu\text{-BzNHC}(CH_2Pyd)_2)_3Cu_3]^{3+}$complexes

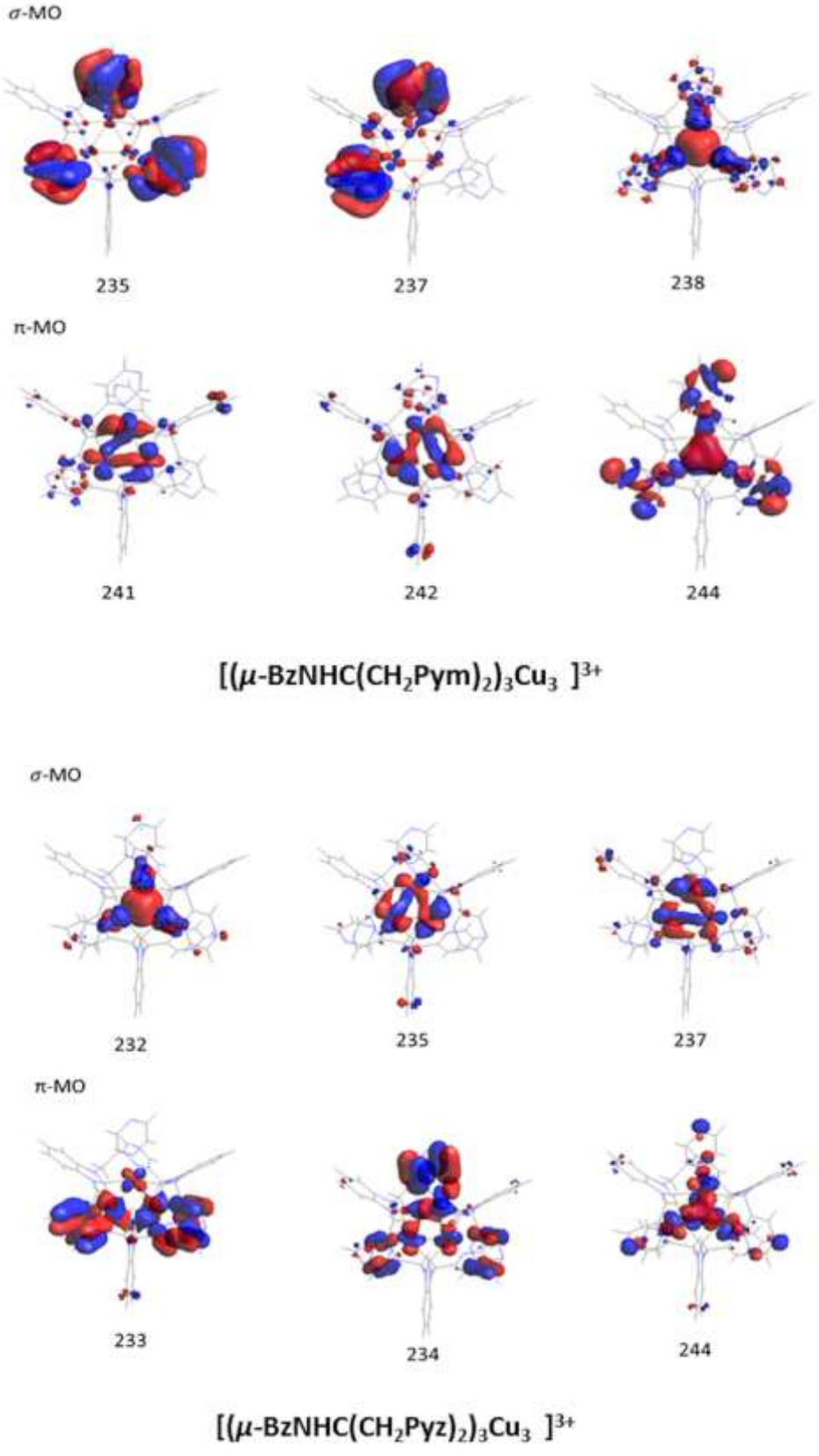


Figure S8: Canonical molecular orbital contribution towards the total NICS (0) with respect to to σ and π molecular orbital of $[(\mu\text{-BzNHC-R}_2)_3Cu_3]^{3+}$ (R= CH_2Pym, CH_2Pyz) complexes.

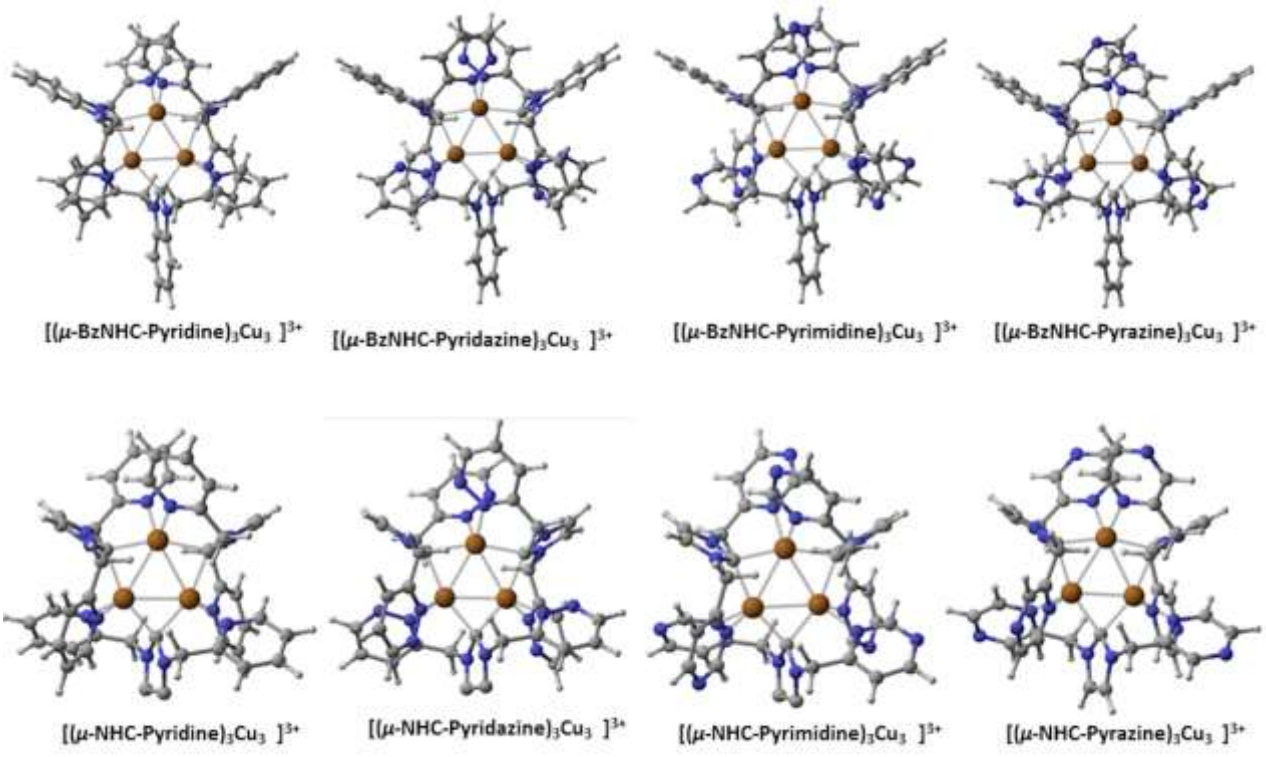


Figure S9: Optimized geometry of $[(\mu\text{-BzNHC-R}_2)_3Cu_3]^{3+}$ (R= CH_2Py, CH_2Pyd, CH_2Pym and CH_2Pyz) and $[(\mu\text{-NHC-R}_2)_3Cu_3]^{3+}$ (R= CH_2Py, CH_2Pyd, CH_2Pym and CH_2Pyz).

Table T1: CMO-NICS(0,1)$_{\sigma zz}$ and CMO-NICS(0,1)$_{\pi zz}$ values computed for the trinuclear Cu(I)-NHC complexes at the B3LYP/LANL2DZ level.

	σ-MO_1	σ-MO_2	σ-MO_3	**NICS(0)$_{\sigma zz}$ (NICS(1)$_{\sigma zz}$)**	π-MO_1	π-MO_2	π-MO_3	**NICS(0)$_{\pi zz}$ (NICS(1)$_{\pi zz}$)**
$[(\mu\text{-BzNHC-(CH2Py)}_2)_3Cu_3]^{3+}$	-2.2 (0.2)	-1.2 (-1.1)	-1.3 (-1.1)	-4.7 (-2.0)	-1.1 (-0.9)	-0.9 (-0.9)	-0.9 (-1.1)	-2.9 (-2.9)
$[(\mu\text{-BzNHC-(CH}_2\text{Pyd)}_2)_3Cu_3]^{3+}$	-2.6 (0.6)	1.0 (0.6)	1.0 (-0.02)	-0.7 (1.2)	1.4 (0.8)	0.1 (0.4)	0.2 (0.3)	1.8 (1.5)
$[(\mu\text{-BzNHC-(CH}_2\text{Pym)}_2)_3Cu_3]^{3+}$	-2.5 (0.1)	-1.7 (1.7)	-1.6 (2.0)	-5.8 (3.8)	0.2 (-1.3)	-0.9 (-1.3)	-0.9 (-0.2)	-1.7 (-2.8)
$[(\mu\text{-BzNHC-(CH}_2\text{Pyz)}_2)_3Cu_3]^{3+}$	-2.8 (-0.02)	-1.6 (-1.3)	-1.6 (-1.3)	-6.1 (-2.6)	-3.6 (0.1)	0.02 (0.2)	0.1 (-1.6)	-3.5 (-1.3)
$[(\mu\text{-NHC-(CH}_2\text{Py)}_2)_3Cu_3]^{3+}$	-2.3 (-0.9)	-0.4 (-0.9)	-0.4 (0.1)	-3.2 (-1.7)	-1.6 (-0.2)	-0.3 (-0.2)	-0.3 (0.3)	-2.2 (-0.1)
$[(\mu\text{-NHC-(CH}_2\text{Pyd)}_2)_3Cu_3]^{3+}$	-2.5 (0.1)	0.3 (-0.1)	0.3 (-0.1)	-2.0 (-0.1)	1.1 (0.1)	-0.1 (0.1)	-0.1 (0.5)	0.9 (0.7)
$[(\mu\text{-NHC-(CH}_2\text{Pym)}_2)_3Cu_3]^{3+}$	-2.6 (-0.6)	-0.4 (-0.5)	-0.4 (-0.02)	-3.4 (-1.1)	0.2 (-0.7)	-0.9 (-0.7)	-0.9 (-0.2)	-1.6 (-1.6)
$[(\mu\text{-NHC-(CH}_2\text{Pyz)}_2)_3Cu_3]^{3+}$	-2.9 (-1.1)	-0.6 (-1.1)	-0.6 (-0.3)	-4.1 (-2.5)	-0.6 (-0.2)	-0.2 (-0.2)	-0.2 (-0.9)	-1.0 (-1.3)
Cu^{3+}	-7.3	-3.6	-3.6	-14.6	-1.2	-2.5	-2.5	-6.2

*The values are in the bracket are correspond to the CMO contributions towards NICS(1).

Table T2. Electronic configuration of Cu_3 inside the complex.

Molecules	**Electronic configuration of Cu inside the complex**
$[(\mu\text{-BzNHC-}(CH_2Py)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.78)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.78)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.78)4p(0.49)5p(0.01)
$[(\mu\text{-BzNHC-}(CH_2Pyd)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.77)4p(0.53)5p(0.01) Cu [core]4S(0.25)3d(9.77)4p(0.53)5p(0.01) Cu [core]4S(0.26)3d(9.77)4p(0.53)5p(0.01)
$[(\mu\text{-BzNHC-}(CH_2Pym)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.78)4p(0.50)5p(0.01) Cu [core]4S(0.25)3d(9.78)4p(0.50)5p(0.01) Cu [core]4S(0.25)3d(9.78)4p(0.50)5p(0.01)
$[(\mu\text{-BzNHC-}(CH_2Pyz)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.78)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.78)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.78)4p(0.49)5p(0.01)
$[(\mu\text{-NHC-}(CH_2Py)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.79)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.79)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.79)4p(0.49)5p(0.01)
$[(\mu\text{-NHC-}(CH_2Pyd)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.26)3d(9.78)4p(0.52)5p(0.01) Cu [core]4S(0.26)3d(9.78)4p(0.52)5p(0.01) Cu [core]4S(0.26)3d(9.78)4p(0.53)5p(0.01)
$[(\mu\text{-NHC-}(CH_2Pym)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.79)4p(0.50)5p(0.01) Cu [core]4S(0.25)3d(9.79)4p(0.50)5p(0.01) Cu [core]4S(0.25)3d(9.79)4p(0.50)5p(0.01)
$[(\mu\text{-NHC-}(CH_2Pyz)_2)_3Cu_3]^{3+}$	Cu [core]4S(0.25)3d(9.79)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.79)4p(0.49)5p(0.01) Cu [core]4S(0.25)3d(9.79)4p(0.49)5p(0.01)

Table T3. Some important distances and angles of the suited M_3 (M=Cu, Ag and Au) tri nuclear cluster complexes with $NHC(CN)_2$) and $NHC(CH_3)_2$ ligands.

Molecule	Distances (Å)		Angle (^{0})		
	(M-M) M=Cu, Ag, Au	(M-C_{nhc}) M=Cu, Ag, Au	(M-M-M) M=Cu, Ag, Au	(M-C_{nhc}-M) M=Cu, Ag, Au	(N-C_{nhc}-N) [Immid]
$[(\mu\text{-}NHC(CN)_2)_3Cu_3]^{3+}$	2.52, 2.52, 2.52	2.09, 2.09, 2.09, 2.09, 2.09, 2.09	60.00, 60.02, 59.98	73.78, 73.80, 73.83	101.88, 101.88, 101.89,
$[(\mu\text{-}NHC(CH_3)_2)_3Cu_3]^{3+}$	2.50, 2.50, 2.50	2.08, 2.08, 2.08, 2.08, 2.08, 2.08	60.00, 60.00, 60.00	73.89, 73.89, 73.88	103.50, 103.50, 103.51
$[(\mu\text{-}NHC(CN)_2)_3Ag_3]^{3+}$	2.89, 2.89, 2.89	2.35, 2.35, 2.35, 2.35, 2.35, 2.35	60.01, 59.99, 59.99	75.88, 75.89, 75.88	102.10, 102.10, 102.10
$[(\mu\text{-}NHC(CH_3)_2)_3Ag_3]^{3+}$	2.86, 2.86, 2.86	2.31, 2.31, 2.31, 2.31, 2.31, 2.31	60.00, 60.00, 60.01	76.32, 76.35, 76.32,	103.78, 103.78, 103.80
$[(\mu\text{-}NHC(CN)_2)_3Au_3]^{3+}$	2.83, 2.83, 2.83	2.26, 2.26, 2.26, 2.26, 2.26, 2.26	60.00, 60.00, 60.00	77.63, 77.63, 77.63	101.86, 101.86, 101.86,
$[(\mu\text{-}NHC(CH_3)_2)_3Au_3]^{3+}$	2.85, 2.85, 2.85	2.25, 2.25, 2.25, 2.25, 2.25, 2.25	60.00, 59.98, 60.01	78.90, 78.90, 78.87	103.42, 103.44, 103.43

Table T4. Some important distances and angles of the suited M_3 (M=Cu, Ag and Au) tri nuclear cluster complexes.

Molecule	Distances (Å)			Angle (^{0})			
	(M-M) M=Cu, Ag, Au	(M-C_{nhc}) M=Cu, Ag, Au	(M-N_{py}) M=Cu, Ag, Au	(M-M-M) M=Cu ,Ag, Au	(M-C_{nhc}-M) M=Cu, Ag, Au	(N_{py}-M-N_{py}) M=Cu, Ag, Au	(N-C_{nhc}-N) [Immid]
$[(\mu\text{-}NHC(CH_2Py)_2)_3Cu_3]^{3+}$ (*exp parameter*)	2.71, 2.71, 2.68 *(2.51, 2.52, 2.51)*	2.05,2.10, 2.13,2.13, 2.10,2.05	2.23,2.17, 2.20,2.20, 2.23,2.18	60.28, 59.39, 60.33 *(60.1, 59.9, 59.9)*	79.67, 79.61, 81.81 *(76.13, 76.31, 75.96)*	94.91, 97.10, 94.91	103.27, 101.83, 103.27
$[(\mu\text{-}BzNHC(CH_2Py)_2)_3Cu_3]^{3+}$	2.47, 2.50, 2.52	2.05,2.01, 2.03,2.02, 2.01,2.04	2.13,2.14, 2.14,2.14, 2.14,2.14,	58.99, 60.85, 60.16	75.97, 75.32, 76.95	93.73, 93.45, 93.60	105.00, 105.24, 105.40
$[(\mu\text{-}NHC(CH_2Py)_2)_3Ag_3]^{3+}$	2.93, 2.93, 2.94	2.34,2.34, 2.34,2.35, 2.34,2.35	2.49,2.49, 2.48,2.48, 2.49,2.50	59.89, 60.21, 59.89	77.82, 77.43, 77.43	95.92, 95.61, 95.60	103.63, 103.64, 103.63
$[(\mu\text{-}BzNHC(CH_2Py)_2)_3Ag_3]^{3+}$	2.94 2.94 2.94	2.37, 2.30, 2.37,2.31, 2.37,2.37	2.51,2.51, 2.51,2.51, 2.51,2.51	50.98, 50.97, 60.01	77.86, 77.90, 77.98	106.43, 105.38, 106.53	105.32, 105.34, 105.34
$[(\mu\text{-}NHC(CH_2Py)_2)_3Au_3]^{3+}$	2.84, 5.28, 5.25	4.45,4.48, 2.22,2.05, 2.20,2.05	2.08,2.08, 2.94,3.30, 3.02,3.30	31.33, 73.81, 74.86	80.01, 101.22, 101.17	170.34, 76.83, 77.80	104.90, 104.87, 103.91
$[(\mu\text{-}BzNHC(CH_2Py)_2)_3Au_3]^{3+}$	2.85, 2.85, 2.85	2.35,2.21, 2.21,2.35, 2.21,2.35	2.52, 2.52, 2.52, 2.52, 2.53, 2.53	59.99, 59.99, 60.02	77.19, 77.23, 77.17	101.26, 101.19, 101.34	105.32, 105.32, 105.35
$[(\mu\text{-}NHC(CH_2Pyz)_2)_3Cu_3]^{3+}$	2.68, 2.68, 2.69,	2.12,2.12, 2.12,2.12, 2.12,2.12	2.22, 2.22, 2.22, 2.22, 2.22, 2.22	59.99, 60.04, 59.97	78.72, 78.74, 78.78	95.34, 95.35, 95.34	103.02, 103.02, 103.02
$[(\mu\text{-}NHC(CH_2Pyz)_2)_3Ag_3]^{3+}$	2.94, 2.94, 2.94	2.35,2.35 2.35,2.35 2.34,2.35	2.51, 2.51, 2.51, 2.51, 2.51, 2.51,	60.00, 60.00, 60.01	77.45, 77.47, 77.40,	95.69, 95.52, 95.55	103.55, 103.44, 103.55
$[(\mu\text{-}NHC(CH_2Pyz)_2)_3Au_3]^{3+}$	2.96, 3.36, 3.27	2.18,2.15, 2.05,3.45, 2.05,3.35	3.19,2.17, 3.47,3.49, 3.05,2.19	64.94, 61.92, 53.13	86.34, 69.81, 70.08	86.27, 84.97, 81.66	104.13, 104.92, 104.94

Table T5. Cartesian coordinates of $[(\mu\text{-NHC-R}_2)_3Cu_3]^{3+}$ (R= CH_2Py, CH_2Pyd, CH_2Pym) and CH_2Pyz) molecules.

1. **$[(\mu\text{-NHC-}(CH_2Py)_2)_3Cu_3]^{3+}$**

Atoms	Coordinates (Angstroms)		
	X	Y	Z
Cu	-1.37563800	-0.71135300	0.00078300
Cu	1.30230000	-0.83450100	-0.00042100
C	-0.11185300	-2.39949300	0.00037600
N	0.03172500	-3.27127600	1.07422000
N	2.63507000	-1.50904800	-1.64020100
N	2.47663400	-1.76816800	1.63563900
C	-2.14289300	-2.41840200	-2.54803000
N	-2.63010500	-1.53217100	-1.63271300
C	2.13526300	1.10301500	0.00423900
C	-3.94879900	-1.19878400	-1.68728200
H	-4.30552500	-0.50929800	-0.93000200
N	-0.33409100	-3.25529300	-1.07290900
N	2.98980300	1.33860800	-1.06716200
C	-0.08942200	-4.60961300	0.67626200
H	0.00476400	-5.43940400	1.35903900
C	-0.33492700	-4.59885900	-0.67406500
H	-0.50436600	-5.41706600	-1.35629000
C	4.05282700	-1.06429600	-3.55314700
H	4.45639800	-0.34980800	-4.26427400
C	3.82072400	-1.55977300	1.69017100
H	4.24041400	-0.90621100	0.93331600
C	-4.82272100	-1.71666800	-2.65676100
H	-5.86824000	-1.42683500	-2.65663300
C	-4.31593500	-2.61732500	-3.61145800
H	-4.96284400	-3.03873300	-4.37492000
C	3.16359600	-0.64126800	-2.55037400
C	-0.66789500	-2.77911000	-2.42603200
H	-0.40792200	-3.55567900	-3.15043000
H	-0.04514300	-1.90246300	-2.63089300
C	-2.95532100	-2.97549700	-3.55042900
H	-2.53862800	-3.67814400	-4.26578000
C	1.90881800	-2.60556200	2.55042300
C	4.05364900	-3.00760500	3.61355400
H	4.65835600	-3.48812100	4.37669000
C	3.00134900	-2.81872900	-1.70097500
H	2.57876500	-3.47514100	-0.94823800
C	0.40674300	-2.82660200	2.42724900
H	0.07415200	-3.57438900	3.15224000
H	-0.13120600	-1.89502000	2.62988100
C	4.15514300	2.00536900	-0.66506200
C	3.88714000	-3.31476400	-2.67107500
H	4.15526400	-4.36605600	-2.67562000
C	2.74321400	0.81725900	-2.42235100
H	1.67306300	0.92281900	-2.62685500
H	3.28802600	1.43189200	-3.14406200
C	4.64240600	-2.15792300	2.65913900

H	5.71048700	-1.96733900	2.65893800
C	4.41874100	-2.42260500	-3.62021400
H	5.10740100	-2.77061500	-4.38413700
C	2.66543000	-3.23674800	3.55257200
H	2.18467900	-3.89767300	4.26750500
N	0.29325500	3.02698300	1.63627300
N	2.81856900	1.65847000	1.08042600
C	1.46599000	3.91974800	3.55849500
H	2.27689800	3.83195100	4.27525400
C	1.30005900	2.95129200	2.55367700
C	-0.55976600	4.08650100	1.69224800
H	-1.33431000	4.12503000	0.93415200
C	4.04026800	2.22042700	0.68564500
C	-0.45510800	5.09441700	2.66436500
H	-1.15455300	5.92381000	2.66495000
C	2.24283700	1.76080200	2.43205100
H	1.70471700	0.82904700	2.63325100
H	3.05489800	1.84664200	3.15912000
C	0.57327900	5.00715700	3.62053600
H	0.68521800	5.76903500	4.38601200
Cu	0.07300100	1.54657500	-0.00046700
C	-2.02227000	1.29590400	-0.00516200
N	-2.64964700	1.91305900	-1.08170100
N	-0.00880100	3.04048300	-1.63816200
C	-3.21015300	-0.34202400	2.55063300
N	-2.76660300	-1.25695800	1.64120100
C	-3.25725700	-2.52524800	1.70197000
H	-2.89964100	-3.21941300	0.94944600
N	-2.85052800	1.61173200	1.06607700
C	-3.81251900	2.58843600	-0.68727400
H	-4.43477000	3.14260200	-1.37234700
C	-3.94730000	2.38585900	0.66362900
H	-4.71405400	2.72215000	1.34377700
C	0.93703100	4.01789800	-1.69340300
H	1.71074300	3.98623600	-0.93417300
C	-4.18745400	-2.93339700	2.67151000
H	-4.55551400	-3.95400300	2.67605000
C	-4.63144600	-1.99401400	3.62012200
H	-5.35117200	-2.27394100	4.38338100
C	-2.65238400	1.06951700	2.42119600
H	-3.13389100	1.73380700	3.14389300
H	-1.57638400	1.07178300	2.62245300
C	-4.13646900	-0.67724100	3.55301500
H	-4.47003500	0.07312100	4.26344900
C	-1.01772100	3.05669900	-2.55625000
C	-0.10545200	5.03711800	-3.62327500
H	-0.14678900	5.80574400	-4.38907100
C	-2.06579000	1.95811700	-2.43301100
H	-2.86579900	2.11531900	-3.16153500
H	-1.61486300	0.98021500	-2.62976700
C	0.92543000	5.03095400	-2.66581900
H	1.69732900	5.79337100	-2.66577200
C	-1.09356300	4.03546000	-3.56188100
H	-1.90841000	4.02157500	-4.27939300
H	4.71222700	2.71323700	1.37064800
H	4.94991500	2.26773000	-1.34559900

2. [(μ-NHC-(CH_2Pyd)$_2$)$_3$$Cu_3$]$^{3+}$

Atoms	Coordinates (Angstroms)		
	X	Y	Z
Cu	1.51280300	-0.14894700	-0.00076400
Cu	-0.88304800	-1.23527300	-0.00189700
C	1.00082100	-2.21107100	-0.01116900
N	1.13671700	-3.09154000	-1.07503100
N	-1.78444900	-2.38492300	1.61387800
N	-1.68268600	-2.45966000	-1.61125100
C	2.98308300	-1.42814300	2.45126200
N	2.96356700	-0.37175700	1.60027800
C	-2.41227400	0.23606600	0.00721900
N	1.58189800	-2.90531300	1.04067700
N	-3.28782400	0.08293600	1.07318600
C	1.77065400	-4.27903900	-0.69310200
H	1.96466500	-5.09105400	-1.37546900
C	2.06051500	-4.15756600	0.63909800
H	2.55075500	-4.84514500	1.30956600
C	-3.42978000	-2.69423600	3.35827600
H	-4.15535300	-2.26719400	4.04363800
C	5.05183200	0.32926900	2.38607800
H	5.84223700	1.06775100	2.30209300
C	5.13159800	-0.74808200	3.29760600
H	5.99763500	-0.86170200	3.94086700
C	-2.69886300	-1.87112600	2.47412500
C	1.76859400	-2.34560000	2.38487800
H	1.87796100	-3.16613300	3.09930200
H	0.86600200	-1.78491600	2.64702600
C	4.06387200	-1.64964200	3.33235000
H	4.06387900	-2.49732700	4.01053700
C	-0.90472100	-3.16219500	-2.47236400
C	-2.83287900	-4.33668500	-3.30761800
H	-3.31975300	-5.06282900	-3.94979700
C	0.58451700	-2.84715300	-2.41310400
H	1.12817400	-3.45803300	-3.13896900
H	0.75130900	-1.79447500	-2.66179000
C	-4.61722000	0.29790500	0.69243000
C	-2.23013100	-4.54381200	2.39521200
H	-1.99342000	-5.59881500	2.30529000
C	-2.87601900	-0.35962800	2.41100200
H	-1.92986000	0.13359800	2.65470500
H	-3.62586300	-0.03712300	3.13865800
C	-3.58681400	-3.57505100	-2.38596600
H	-4.66176100	-3.68915400	-2.29301700
C	-3.19316200	-4.07137000	3.31571800
H	-3.72472100	-4.76357500	3.95993600
C	-1.45273200	-4.11925000	-3.35409400
H	-0.81760100	-4.67034500	-4.04071100
N	-1.28717800	2.66816900	-1.62899000
N	-3.25864100	0.55969500	-1.04372300
C	-2.86035100	3.29914200	-3.35271400
H	-3.67087600	3.02803000	-4.02215200

C	-2.30374700	2.34892600	-2.46896200
C	-4.59770400	0.60839700	-0.64055100
C	-1.28227200	4.86469700	-2.43341900
H	-0.82716600	5.84699400	-2.36164100
C	-2.79104300	0.90770000	-2.39125800
H	-1.97471300	0.22736400	-2.65299600
H	-3.60666500	0.74802200	-3.10179800
C	-2.33915400	4.59606300	-3.33257500
H	-2.72447100	5.37781700	-3.97841000
Cu	-0.62615700	1.38730500	-0.00540200
C	1.41322400	1.97421600	0.02693400
N	1.71174000	2.80116700	1.10092200
N	-1.18407400	2.75087800	1.59412500
C	3.20682000	0.83757200	-2.44651500
N	2.96692900	-0.20912200	-1.61753100
N	2.12969600	2.54776700	-1.01336300
C	2.57127100	3.84302800	0.73471500
H	2.91540400	4.59531700	1.42625000
C	2.84285500	3.67711500	-0.59666100
H	3.46536300	4.25926700	-1.25710600
C	4.87505500	-1.30411500	-2.41192700
H	5.49795800	-2.18965300	-2.34128400
C	5.17908400	-0.24731700	-3.29984400
H	6.05518900	-0.29907300	-3.93741300
C	2.20187500	1.97920300	-2.36491000
H	2.47278800	2.77090100	-3.06868500
H	1.20543000	1.61330300	-2.63110500
C	4.31615800	0.85213000	-3.32001500
H	4.49229200	1.69519600	-3.98094100
C	-0.29278600	3.27688400	2.47130300
C	-1.95429600	4.81571000	3.28681100
H	-2.29328900	5.62300600	3.92718200
C	1.10146700	2.66432100	2.42898200
H	1.74742300	3.14422500	3.16925800
H	1.04334800	1.59763400	2.66684900
C	-2.83291500	4.22769500	2.34869800
H	-3.86045100	4.55884600	2.24083600
C	-0.64801800	4.32187900	3.35172500
H	0.07487000	4.72965300	4.05157600
N	-0.76111300	3.92827200	-1.60374900
N	-3.03346600	-2.65385200	-1.56000000
N	-1.53554600	-3.72674300	1.56627600
N	3.79556000	-1.29451400	-1.59260300
N	3.99534400	0.52191900	1.55913400
N	-2.46567700	3.21669200	1.52380200
H	-5.40759600	0.84875400	-1.31055600
H	-5.44753200	0.21989900	1.37590400

3. [(μ-NHC-(CH_2Pym)$_2$)$_3$$Cu_3$]$^{3+}$

Atoms	Coordinates (Angstroms)		
	X	**Y**	**Z**
Cu	1.31585400	-0.80380000	0.00007500
Cu	0.03876200	1.54122900	-0.00229700
C	2.12446700	1.15703300	0.00353200
N	2.79173000	1.73992200	1.07762800
N	-0.06878800	3.02433200	-1.63551800
N	0.21947200	3.01540500	1.63447000
C	3.19744000	-0.57717300	-2.53863200
N	2.65667500	-1.44784900	-1.63408200
C	-2.06417100	1.26079200	-0.00910700
C	3.03590500	-2.75297300	-1.71992800
H	2.62604000	-3.44288700	-0.99165800
N	2.98179600	1.40479800	-1.06522700
N	-2.70092200	1.87484800	-1.08407400
C	4.00348000	2.32668200	0.68368500
H	4.66407800	2.83639500	1.36759000
C	4.12916500	2.10463900	-0.66317700
H	4.91903700	2.38580100	-1.34212400
C	-1.13944700	4.04744400	-3.53631900
H	-1.94125200	4.08442800	-4.26595100
C	-0.67089000	4.04242600	1.71835300
H	-1.46651500	4.07717500	0.98339500
C	4.41387900	-2.40038800	-3.53878100
H	5.09925000	-2.82019600	-4.26863700
C	-1.08481400	3.05023800	-2.54962100
C	2.76883600	0.87941200	-2.42353500
H	3.32621400	1.49519100	-3.13434600
H	1.70314900	0.96914100	-2.65848000
C	4.09491200	-1.02537000	-3.52080300
H	4.53601600	-0.34646000	-4.24270800
C	1.23666600	2.99132800	2.54725200
C	0.35796200	4.99678800	3.55204000
H	0.37119000	5.79570500	4.28703800
C	0.86878500	4.00868400	-1.71528900
H	1.66313600	4.00487100	-0.97816400
C	2.22752100	1.84069400	2.43320100
H	3.04302900	1.97107000	3.14947300
H	1.72267800	0.89598600	2.66048200
C	-3.88245100	2.52105500	-0.69136400
C	-2.12942400	1.94789200	-2.43826200
H	-1.66886800	0.98032500	-2.66326500
H	-2.93599300	2.11611000	-3.15676100
C	-0.11098700	5.01440900	-3.54833900
H	-0.08542400	5.81468100	-4.28153700
C	1.33967600	3.98252300	3.53616700
H	2.14329400	3.97986700	4.26473600
N	-2.72483000	-1.31166900	1.63540100
N	-2.90807700	1.55219700	1.05899600
C	-4.13913700	-0.81175600	3.52142900
H	-4.54468200	-0.10935300	4.24170100
C	-3.22035100	-0.41242900	2.53790000

C	-3.16970400	-2.59565800	1.72486300
H	-2.79557500	-3.30757200	0.99855900
C	-4.01953900	2.30704300	0.65573600
C	-2.71836900	1.01999900	2.41811100
H	-1.64836200	1.05515500	2.64815900
H	-3.24072200	1.66532500	3.12931300
C	-4.52750800	-2.16878100	3.54307800
H	-5.23294500	-2.55141800	4.27425000
Cu	-1.35404200	-0.73826400	-0.00157600
C	-0.06014500	-2.41841000	0.00026200
N	-0.27288400	-3.28219800	-1.07091900
N	-2.58302900	-1.57983500	-1.63271200
C	1.97061300	-2.57399600	2.54490900
N	2.50005000	-1.70049200	1.63650000
C	3.83468300	-1.44374300	1.72135000
H	4.26275600	-0.76892600	0.98936800
N	0.11024600	-3.29031800	1.07235900
C	-0.24113700	-4.62673100	-0.67208700
H	-0.39206400	-5.44962700	-1.35325800
C	0.01278500	-4.63217300	0.67502800
H	0.12322600	-5.46073600	1.35710200
C	-3.90390100	-1.25920600	-1.71513700
H	-4.29775900	-0.56528900	-0.98179400
C	4.14706600	-2.82163300	3.54765600
H	4.83241900	-3.23669100	4.28024100
C	0.47875000	-2.85583700	2.42944100
H	0.18297400	-3.62922100	3.14324100
H	-0.08652400	-1.94659900	2.65920200
C	2.77769500	-3.16421400	3.53041900
H	2.37368500	-3.86245600	4.25558900
C	-2.09738100	-2.47719600	-2.54227900
C	-4.28467800	-2.61893900	-3.54202500
H	-4.99021300	-2.99982300	-4.27402000
C	-0.62087300	-2.83158600	-2.42820400
H	-0.36422000	-3.61930900	-3.14149400
H	-0.01167600	-1.95152200	-2.65948000
C	-2.93333000	-3.02702200	-3.52713300
H	-2.56448800	-3.74335800	-4.25340500
N	0.89278300	4.99516300	-2.63325300
N	-4.04246200	-3.06064700	2.64056100
N	3.88394700	-3.26415800	-2.63418000
N	-0.64730900	5.02654600	2.63883100
N	4.67542700	-1.96147700	2.63864400
N	-4.76989100	-1.73524500	-2.63150800
H	-4.79475600	2.62774400	1.33403600
H	-4.51662500	3.06225800	-1.37606600

4. [(μ-NHC-($CH_2Pyz)_2)_3Cu_3$]$^{3+}$

Atoms	Coordinates (Angstroms)		
	X	Y	Z
N	1.53595800	2.90034000	1.07245100
N	1.85055400	2.71053800	-1.07460300
N	1.74355000	-2.78043400	1.07338000
N	3.04954100	0.09313400	-1.63405000
C	3.97683000	-1.34517700	3.54429600
C	1.16471400	-2.11088800	-0.00034000
C	2.33879800	-3.98601900	0.67519800
N	-1.33827400	2.73807600	1.63580500
N	3.04228800	-0.21036900	1.63581400
C	-0.43220000	3.19958300	2.54499800
C	1.92202200	2.13689500	-2.42987700
C	2.98922900	-1.22631000	2.54439600
C	3.03592300	1.10902700	-2.54415500
C	2.28130800	4.01917500	0.67397700
C	2.49170700	3.89223600	-0.67624500
C	4.05803600	-0.81537400	-1.71655200
C	4.02722200	1.18801900	-3.54429900
C	1.24601300	2.06387800	-0.00104900
C	4.08570600	0.65784300	1.71917600
C	5.07092000	0.52038600	2.71815700
C	0.99670100	2.69462200	2.42814000
C	1.83660400	-2.21049100	2.42886500
C	-2.61238000	3.20579900	1.72056500
C	5.04772700	-0.71783200	-2.71588500
C	-0.82360400	4.11249400	3.54628600
C	-2.98668700	4.12575200	2.72119100
N	1.42195200	-2.95829100	-1.07365500
C	-0.98439000	-4.08301400	-3.54284700
C	2.12344600	-4.10507000	-0.67490200
N	-1.44434600	-2.68502600	-1.63574200
C	-0.55726100	-3.18322000	-2.54424300
C	-2.73562900	-3.10352600	-1.71826700
C	-3.14580200	-4.01104600	-2.71608900
C	0.89027000	-2.73363800	-2.42934200
N	-3.27288100	0.24798800	-1.07534900
N	-3.28050200	-0.11973700	1.07156700
N	-1.70291200	-2.52800900	1.63497500
N	-1.60532500	2.59504100	-1.63333600
C	-2.47817000	2.07597100	-2.54391300
C	-2.83353800	-0.48455500	2.42732700
C	-2.55698900	-1.97464800	2.54322100
C	-4.61694800	0.21312200	-0.67719900
C	-4.62203800	-0.03354900	0.67278700
C	-1.47247500	-3.86568100	1.71804100
C	-3.15487400	-2.77112500	3.54191300
C	-2.41080000	0.04736100	-0.00165400
C	-2.81181600	0.59727100	-2.43043400
C	-1.32222900	3.92264600	-1.71482400
C	-2.08516700	-4.65085500	2.71589700
C	-3.04197100	2.89590000	-3.54344300

C	-1.90083200	4.73168400	-2.71392000
H	-0.11875800	4.48629100	4.28354900
H	-3.99902700	4.51092500	2.78842900
H	-3.32866300	2.85263700	0.98829000
H	1.03666600	1.62260200	2.64640900
H	1.63701600	3.20974700	3.14961400
H	2.59537400	4.79445000	1.35567000
H	3.03074200	4.53177300	-1.35801400
H	-0.64239800	4.33895300	-0.98093700
H	-1.68736300	5.79371500	-2.77886000
H	-3.73355100	2.50032000	-4.28188700
H	-3.58913900	0.33141400	-3.15220100
H	-1.92602200	-0.00719800	-2.65048200
H	-5.44011500	0.36086400	-1.35907300
H	-5.45060800	-0.14926000	1.35431500
H	-3.60046200	-0.18798300	3.14828000
H	-1.92526300	0.08592400	2.64679600
H	-3.83290100	-2.34835200	4.27786700
H	-1.91363900	-5.72040100	2.78192500
H	-0.80751600	-4.30911300	0.98646200
H	1.50963900	-3.27464700	-3.15017200
H	0.97188800	-1.66441600	-2.64982200
H	2.40708700	-4.89205500	-1.35650800
H	2.85262400	-4.64582400	1.35713300
H	-0.29506400	-4.48587900	-4.27947300
H	-4.17231000	-4.35696200	-2.78184600
H	-3.43715000	-2.72110600	-0.98637900
H	4.13833000	1.45452800	0.98667100
H	5.91166000	1.20337000	2.78443200
H	3.94872800	-2.14303800	4.28098200
H	0.88869600	-1.70885800	2.64874500
H	1.96327400	-3.02269700	3.15007700
H	4.07913700	-1.61286300	-0.98334600
H	5.86080100	-1.43358400	-2.78154900
H	4.02941000	1.98481800	-4.28266600
H	0.95569800	1.67170500	-2.64945900
H	2.07988400	2.94316000	-3.15162000
Cu	1.55058900	-0.03033000	-0.00044400
Cu	-0.80056700	-1.32616900	-0.00096600
Cu	-0.74907200	1.35743200	-0.00051500
N	-2.75426800	4.21777100	-3.63230000
N	-2.91992800	-4.10331800	3.63195500
N	5.02861500	0.27850500	-3.63391700
N	-2.09524500	4.57349600	3.63807100
N	5.01292400	-0.47559300	3.63494500
N	-2.27291900	-4.49495700	-3.63247700

Table T6: Cartesian coordinates of $[(\mu\text{-BzNHCR}_2)_3\ Cu_3]^{3+}$ (R= CH_2Py, CH_2Pyd, CH_2Pym and CH_2Pyz) molecules.

1. **$[(\mu\text{-BzNHC-}(CH_2Py)_2)_3Cu_3]^{3+}$**

Atoms	Coordinates (Angstroms)		
	X	**Y**	**Z**
N	-2.73597300	1.75739300	-1.09278300
N	-2.91715400	1.45876800	1.07826000
N	-0.17014600	-3.25090700	-1.08240000
N	-2.66762200	-1.40122300	1.65562100
C	-2.82585900	-3.09110600	-3.53165300
C	0.01387100	-2.40055500	0.00012600
N	-0.15788000	3.02907800	-1.62941100
N	-2.56288500	-1.65067400	-1.60402400
C	-1.15618200	2.98000000	-2.55795100
C	-2.66820900	0.92843600	2.42536500
C	-2.03514500	-2.50012600	-2.53174600
C	-3.15098500	-0.50941200	2.56783500
C	-3.08289500	-2.69538800	1.72506600
C	-4.46279100	-2.23705800	3.65757500
C	-4.04361200	-0.89483600	3.58235500
C	-2.08814300	1.19099600	-0.00300200
C	-3.89786900	-1.38935300	-1.64212400
C	-4.75144400	-1.94688900	-2.60757300
C	-2.13737900	1.82102300	-2.43247300
C	-4.20488900	-2.80939400	-3.57531200
C	-0.54025700	-2.77346800	-2.42152300
C	0.73268000	4.05683700	-1.68177100
C	-3.97720000	-3.15265900	2.70615300
C	-1.27419300	3.94487100	-3.57253900
C	-0.34446600	5.00091700	-3.63040300
C	0.67419500	5.06074200	-2.66181100
N	0.20820800	-3.24693000	1.08389500
C	2.86076900	-3.05448500	3.53342800
N	2.58231300	-1.62113600	1.60251700
C	2.06387400	-2.47402300	2.53228900
C	3.91441800	-1.34558900	1.63981600
C	4.77398200	-1.89204300	2.60631600
C	4.23680400	-2.75819200	3.57610200
C	0.57195300	-2.76260200	2.42212700
N	2.71706100	1.78685500	1.09167200
N	2.89908700	1.49217200	-1.07976900
N	2.68197100	-1.36922800	-1.65827500
N	0.12371600	3.02679700	1.63377600
C	1.12466200	2.98959900	2.56009300
C	2.65541500	0.96071700	-2.42726900
C	3.15324200	-0.47185500	-2.57133200
C	3.11130900	-2.65878200	-1.72911100
C	4.48095300	-2.18483200	-3.66502700
C	4.04737300	-0.84729900	-3.58828600
C	2.07375500	1.21492800	0.00208700
C	2.12006700	1.84303600	2.43240400

C	-0.77994700	4.04307300	1.68980300
C	4.00805600	-3.10596900	-2.71258800
C	1.23281200	3.95490300	3.57541200
C	0.28968400	4.99866800	3.63695600
C	-0.73215000	5.04625800	2.67110100
H	-2.07736300	3.87843300	-4.30010300
H	-0.42041900	5.76041100	-4.40269400
H	1.40231000	5.86500100	-2.65930600
H	1.49997000	4.07288800	-0.91575800
H	-1.62143500	0.87178400	-2.60944100
H	-2.93232000	1.91327100	-3.17709700
H	-1.54940900	4.05064000	0.92583700
H	-1.47070600	5.84094700	2.67138600
H	0.35777100	5.75822800	4.40991700
H	2.03865400	3.89799800	4.30084600
H	2.91506500	1.94556000	3.17551300
H	1.61643200	0.88754500	2.61090500
H	3.14217100	1.60812500	-3.16124300
H	1.57661000	1.00221900	-2.60800000
H	4.40272300	-0.11139800	-4.30321500
H	5.17576000	-2.49536600	-4.43952700
H	4.32755300	-4.14268400	-2.72497300
H	2.73076400	-3.33920700	-0.97549700
H	0.27189000	-3.50473000	3.16639600
H	-0.00097100	-1.84915100	2.61115300
H	2.41972700	-3.72800600	4.26200700
H	4.87212200	-3.19982100	4.33791600
H	5.83111600	-1.64860500	2.59262400
H	4.29374200	-0.67897500	0.87324600
H	-4.28434200	-0.72531400	-0.87686900
H	-5.81108200	-1.71456300	-2.59461400
H	-4.83528400	-3.25938200	-4.33632600
H	-2.37775400	-3.76163600	-4.25869000
H	0.02375500	-1.85515500	-2.61384700
H	-0.23369000	-3.51466800	-3.16405900
H	-2.69291800	-3.37145100	0.97233500
H	-4.28511700	-4.19288400	2.71755300
H	-5.15617700	-2.55546800	4.43013600
H	-4.40875300	-0.16298000	4.29648900
H	-1.58976700	0.98072600	2.60573900
H	-3.16137700	1.57019200	3.16004900
Cu	-1.33127200	-0.77696000	0.00966800
Cu	1.33873700	-0.76146800	-0.01093000
Cu	-0.00950700	1.54393700	0.00062100
C	0.31019500	-5.80157000	1.41868300
C	0.17811100	-7.00137400	0.70034700
H	0.52216800	-5.81729100	2.48319100
C	-0.24165900	-5.80706000	-1.41301000
C	-0.09531400	-7.00410600	-0.69284600
H	0.28720900	-7.94864800	1.21962000
H	-0.45371900	-5.82689200	-2.47743400
H	-0.19328800	-7.95342300	-1.21060000
C	-5.18352100	2.64579900	1.39948500
C	-6.15996100	3.34659100	0.67243800
C	-6.02834700	3.56511000	-0.72420200
C	-4.91797100	3.08658000	-1.43916700

H	-5.30060600	2.48552700	2.46675500
H	-7.03529000	3.73035200	1.18758700
H	-6.80402500	4.11453100	-1.24892100
H	-4.83181500	3.26442800	-2.50658200
C	5.15396400	2.70074900	-1.40175000
C	4.88599300	3.13737600	1.43729000
C	5.99131000	3.62688000	0.72194700
C	6.12416300	3.41029400	-0.67488400
H	5.27189100	2.54221500	-2.46918000
H	4.79851700	3.31407100	2.50478000
H	6.76198000	4.18351200	1.24645500
H	6.99548400	3.80266600	-1.19034100
C	0.15918100	-4.60522800	0.69696200
C	-0.10459000	-4.60790900	-0.69320300
C	3.91913000	2.42360400	0.70904600
C	4.04718800	2.21529400	-0.68471800
C	-3.94465400	2.38181700	-0.71073100
C	-4.07171100	2.17138500	0.68288500

2. [(μ-BzNHC-(CH_2Pyd)$_2$)$_3$$Cu_3$]$^{3+}$

Atoms	**Coordinates (Angstroms)**		
	X	**Y**	**Z**
Cu	1.31253000	0.75227000	-0.00380500
Cu	-1.30711800	0.76163800	0.00363700
Cu	-0.00547600	-1.51494000	-0.00000700
N	2.56413000	1.52757500	1.58075400
N	-2.59184800	1.44670200	1.60561800
N	2.60217500	1.42765900	-1.60601400
N	-0.06409400	-2.97576700	-1.59499500
N	-2.55272200	1.54566900	-1.58100900
N	0.04237300	-2.97596800	1.59504100
N	0.25816400	3.27384800	1.06773800
N	-2.96231600	-1.41956400	1.06703000
N	2.95221800	-1.44097500	-1.06676700
N	-2.72067400	-1.83488000	-1.07130300
N	-0.23441100	3.27569900	-1.06785500
N	2.70743600	-1.85431100	1.07157200
C	0.00886300	2.42615600	-0.00008900
C	-2.10448100	-1.20679900	-0.00046800
C	2.09579000	-1.22201700	0.00059100
C	-4.10083300	-2.15785500	0.68208800
C	0.18163700	4.62968700	0.68633800
C	4.08543900	-2.18729000	-0.68166100
C	-0.14831700	4.63092800	-0.68629900
C	-3.93869100	-2.43699800	-0.69232900
C	3.92120900	-2.46509000	0.69279100
C	-4.89303600	-3.17657200	-1.40920000
C	-0.32032800	5.82825500	-1.39950700
C	4.87024700	-3.21125500	1.40986400
C	-0.14334000	7.02699600	-0.68903200
C	-6.02123500	-3.62210200	-0.70074100

C	5.99531600	-3.66485300	0.70155000
C	-6.18639800	-3.33758200	0.67952000
C	0.19313300	7.02574000	0.68941500
C	6.16261800	-3.38168200	-0.67873200
C	0.36189300	5.82570800	1.39971600
C	-5.22800200	-2.59943500	1.39351200
C	5.20954200	-2.63687600	-1.39292100
C	-2.75776100	-0.84589200	2.39901400
C	0.66325600	2.80931600	2.39641100
C	2.75168600	-0.86621700	-2.39889200
C	2.15054400	2.48178400	2.45159000
C	-3.21746100	0.60521400	2.46580300
C	3.22172500	0.58153800	-2.46602100
C	-4.21928200	1.06274000	3.34901100
C	3.05119300	3.11471600	3.33546500
C	4.22678600	1.03167700	-3.34935000
C	-3.87475800	3.23928300	2.38250000
C	4.76235900	1.74320000	2.34514700
C	3.89800200	3.21080300	-2.38316100
C	-2.11669100	-1.95041700	-2.40065600
C	-0.64292600	2.81416300	-2.39651900
C	2.10239300	-1.96550900	2.40079800
C	-2.13247200	2.49706300	-2.45172600
C	-1.10121300	-3.08473600	-2.46229200
C	1.07871000	-3.09246000	2.46230500
C	-1.21229800	-4.17971600	-3.34644500
C	-3.02868400	3.13633200	-3.33554900
C	1.18189500	-4.18823900	3.34640600
C	0.82762000	-4.99466100	-2.36409700
C	-4.74936900	1.77656000	-2.34553100
C	-0.86392500	-4.98836200	2.36410500
H	-0.57808800	5.84872400	-2.45410200
H	-4.78424500	-3.40332100	-2.46553500
H	4.75975100	-3.43704900	2.46622300
H	-6.78410800	-4.19629900	-1.21777800
H	-0.26597000	7.97559800	-1.20296400
H	6.75408700	-4.24433400	1.21873000
H	0.32224000	7.97340200	1.20349400
H	-7.07287000	-3.69882800	1.19201400
H	7.04659400	-3.74920500	-1.19107700
H	-5.37102400	-2.39126600	2.44960300
H	0.61979000	5.84425500	2.45431600
H	5.35412300	-2.42977800	-2.44900800
H	0.41728100	3.57675600	3.13473400
H	-3.29516500	-1.44893300	3.13538900
H	3.28470700	-1.47321100	-3.13520100
H	-1.68970400	-0.90263300	2.63181400
H	0.08076900	1.91416200	2.63629100
H	1.68322800	-0.91541100	-2.63154200
H	2.70606400	3.87248000	4.03186500
H	-4.70883400	0.37961600	4.03603300
H	4.71132800	0.34492200	-4.03629800
H	5.78676800	1.40071800	2.24338000
H	-4.08611500	4.29950700	2.29089400
H	4.11702800	4.26948300	-2.29169700
H	-0.06691700	1.91486200	-2.63656300

H	-1.62130900	-1.00205300	-2.63158500
H	1.61371000	-1.01364500	2.63160100
H	-2.90560300	-2.10640800	-3.14104200
H	-0.39159000	3.57992500	-3.13477100
H	2.89002500	-2.12711700	3.14133900
H	-2.67835700	3.89182400	-4.03182600
H	-2.04460500	-4.25191700	-4.03955400
H	2.01373400	-4.26656100	4.03940400
H	-5.77612700	1.44113600	-2.24389400
H	1.63024900	-5.71803400	-2.26586200
H	-1.67180500	-5.70588300	2.26596100
C	-4.56214100	2.41719100	3.30433800
H	-5.32890300	2.83493900	3.94800200
C	-0.22292000	-5.16595300	-3.29406200
H	-0.25039000	-6.03861800	-3.93786100
H	5.34909000	2.79576300	-3.94870900
H	0.20655400	-6.04012500	3.93781700
C	0.18538600	-5.16727100	3.29403500
C	4.57937000	2.38364700	-3.30494400
C	4.39642600	2.73910400	3.27907100
C	-4.37647500	2.76999700	-3.27932500
H	5.14391100	3.19049200	3.92270700
H	-5.12077100	3.22660300	-3.92297600
N	-0.94271100	-3.91875200	1.53594000
N	2.92881300	2.75183800	-1.55487600
N	3.87246800	1.14425400	1.51723900
N	-3.86369200	1.17143300	-1.51759800
N	0.91409400	-3.92569600	-1.53587600
N	-2.90892800	2.77318800	1.55426100

3. [(μ-BzNHC-(CH_2Pym)$_2$)$_3$$Cu_3$]$^{3+}$

Atoms	Coordinates (Angstroms)		
	X	**Y**	**Z**
Cu	1.49438400	-0.34979900	0.00670100
Cu	-1.05429400	-1.12019900	-0.00509100
Cu	-0.45000600	1.47076600	-0.00230800
N	2.91126800	-0.81341500	-1.61951600
N	-2.15630500	-2.09622100	-1.64418000
N	2.95939300	-0.55599400	1.64172000
N	-1.00611500	2.84572100	1.62827700
N	-1.97189800	-2.30016500	1.61495800
N	-0.74167000	2.92398100	-1.63235000
N	1.13044000	-3.07028500	-1.08320700
N	-3.23229500	0.56924300	-1.07782400
N	2.36945700	2.25873100	1.08606800
N	-3.14073600	0.91906700	1.08980000
N	0.76948300	-3.18227900	1.08153800
N	2.10300600	2.50658000	-1.08080800
C	0.69985900	-2.31273800	-0.00037200
C	-2.35749900	0.55202700	0.00194200
C	1.65406900	1.76217200	0.00326200

C	-4.54338600	0.92965800	-0.68306500
C	1.47537400	-4.38769900	-0.69598800
C	3.25887800	3.28940200	0.69712500
C	1.22707500	-4.46469600	0.69342000
C	-4.48048400	1.17156400	0.70832700
C	3.07474900	3.46063200	-0.69395400
C	-5.61334600	1.57006300	1.43806200
C	1.44746300	-5.64956300	1.41612400
C	3.79597300	4.42443200	-1.41904700
C	1.93172900	-6.75315200	0.69593600
C	-6.81310400	1.71237100	0.72289100
C	4.71264800	5.20704900	-0.69925300
C	-6.87702000	1.46597900	-0.67412600
C	2.18450500	-6.67480900	-0.69923400
C	4.89973700	5.03310100	0.69758600
C	1.96117700	-5.49035700	-1.41918400
C	-5.74321800	1.06950700	-1.40108700
C	4.17655900	4.07062600	1.41986100
C	-2.86141900	0.12475900	-2.42618700
C	1.33746600	-2.51785500	-2.42667600
C	2.30617700	1.67671500	2.43137100
C	2.67312300	-1.79500900	-2.54025400
C	-2.89705400	-1.39259600	-2.55253100
C	3.18270800	0.43739400	2.55392100
C	-3.63488000	-2.05704800	-3.54492000
C	3.62224400	-2.09605500	-3.52981300
C	4.16609800	0.29335200	3.54515500
C	-2.59865200	1.15709600	2.43237100
C	0.28404100	-2.84489400	2.42451600
C	1.52482200	2.40497300	-2.42534700
C	-1.22844100	-2.98975800	2.53177700
C	-1.96892900	2.53893400	2.54869200
C	0.23442400	3.20446000	-2.54745300
C	-2.33419100	3.46347900	3.53987600
C	-1.85054000	-3.77604700	3.51429200
C	0.02897500	4.17485100	-3.54068800
H	1.26190300	-5.72907600	2.48270400
H	-5.58539900	1.76099400	2.50631300
H	3.66801900	4.57129100	-2.48693200
H	-7.71349900	2.01674000	1.24745200
H	2.11836400	-7.68813700	1.21506000
H	5.29290200	5.96255300	-1.21987700
H	2.55828600	-7.55181500	-1.21852400
H	-7.82473300	1.58790300	-1.18938800
H	5.61845700	5.65989500	1.21631500
H	-5.81223300	0.88747900	-2.46902000
H	2.15863100	-5.45115000	-2.48587700
H	4.33260800	3.95432300	2.48779900
H	1.27761500	-3.32511800	-3.16086100
H	-3.53557100	0.58313900	-3.15388100
H	2.60613500	2.42988000	3.16408200
H	-1.84805800	0.48391100	-2.63466600
H	0.52361400	-1.81478000	-2.63307200
H	1.26478800	1.40545100	2.63325100
H	3.44960800	-2.87303100	-4.26665000
H	-4.22945200	-1.51416200	-4.27162000

H	4.35758300	1.07237000	4.27513300
H	0.56670900	-1.80869700	2.63808700
H	-1.84010800	0.39272600	2.63178100
H	1.31747200	1.34836000	-2.62479200
H	-3.39673700	1.03869000	3.16951700
H	0.78066000	-3.48548900	3.15746300
H	2.25744400	2.74877100	-3.15975200
H	-1.27559000	-4.33083100	4.24776500
H	-3.09737000	3.23673800	4.27642100
H	0.79341900	4.41124500	-4.27290500
C	-3.58370800	-3.46707200	-3.56688400
H	-4.12904900	-4.04884400	-4.30366500
C	-1.67621600	4.71201500	3.54614600
H	-1.90718300	5.47760500	4.28047200
H	5.68675000	-1.08798700	4.29757900
H	-1.44344200	5.60740700	-4.29353500
C	-1.21324100	4.84422500	-3.55646100
C	4.90943200	-0.90596600	3.56179300
C	4.82277800	-1.35433100	-3.53379300
C	-3.26070000	-3.82857000	3.51650100
H	5.60372700	-1.53226100	-4.26671800
H	-3.81099400	-4.41720400	4.24409000
C	3.73441300	-1.67213700	1.72775600
C	-1.90334100	3.62899000	-1.71848700
C	-3.32611000	-2.42014900	1.68809200
C	4.10307600	-0.15966800	-1.69362600
C	-2.17765800	-3.45450500	-1.73557400
C	-0.43499600	4.07905100	1.70497800
H	3.57185400	-2.45465000	0.99608400
H	-2.67339300	3.41965300	-0.98549000
H	0.31594300	4.33100800	0.96553400
H	-1.60585400	-4.01586800	-1.00620100
H	4.30209800	0.60683100	-0.95402100
H	-3.91793600	-1.88778800	0.95291600
N	4.69396600	-1.88894200	2.64956700
N	-2.17981000	4.57130600	-2.64205000
N	5.06361500	-0.38609900	-2.61188600
N	-3.99885500	-3.15021900	2.59997700
N	-0.72657200	5.02014100	2.62497200
N	-2.85480700	-4.16622600	-2.65859000

4. [(μ-BzNHC-(CH_2Pyz)$_2$)$_3$$Cu_3$]$^{3+}$

Atoms	Coordinates (Angstroms)		
	X	**Y**	**Z**
Cu	1.51880800	-0.25180100	0.00289400
Cu	-0.98088500	-1.19003600	-0.00341500
Cu	-0.54694600	1.44628800	0.00382100
N	2.96962200	-0.62499200	-1.62914800
N	-2.02796500	-2.24976400	-1.63922000
N	3.01753600	-0.36460700	1.62801800
N	-1.19963900	2.79094900	1.63128700
N	-1.82847000	-2.43718100	1.61683300
N	-0.94084200	2.89443300	-1.62336900
N	1.31840400	-2.98759900	-1.08110800
N	-3.24737700	0.36009500	-1.08323400
N	2.20687900	2.40250100	1.08846600
N	-3.18964900	0.70521500	1.08738500
N	0.97706100	-3.11211800	1.08722900
N	1.93083900	2.62944700	-1.08083700
C	0.84697500	-2.25576900	0.00133900
C	-2.38052100	0.39677700	0.00137900
C	1.52842400	1.86159500	0.00413100
C	-4.58118600	0.62842900	-0.69338700
C	1.74932600	-4.27781800	-0.68980500
C	3.03099100	3.48545200	0.69962700
C	1.51104700	-4.36485100	0.70192200
C	-4.54058200	0.87147900	0.69989200
C	2.83776000	3.64426100	-0.69299900
C	-5.70040900	1.19620300	1.42468700
C	1.80488700	-5.53236100	1.42771000
C	3.49523500	4.65380700	-1.41732700
C	2.35583500	-6.60599100	0.70944800
C	-6.90422000	1.25819300	0.70411700
C	4.36107500	5.49237900	-0.69672400
C	-6.94651300	1.00458700	-0.69284500
C	2.60360700	-6.51540800	-0.68629400
C	4.56148800	5.32770400	0.69983300
C	2.30471800	-5.34968500	-1.41015300
C	-5.78569300	0.68526600	-1.41588900
C	3.89988800	4.32140200	1.42230400
C	-2.83252800	-0.05966200	-2.42828700
C	1.48351500	-2.42019500	-2.42597900
C	2.17793700	1.80654800	2.43071300
C	2.76846000	-1.61614700	-2.54406000
C	-2.78099400	-1.57385900	-2.55387400
C	3.14148300	0.63618000	2.54639700
C	-3.47380500	-2.27193500	-3.56417400
C	3.72672700	-1.86710400	-3.54754700
C	4.13023200	0.56666100	3.54913500
C	-2.69936900	-4.29000400	-2.73552700
C	5.07995000	-0.18588600	-2.71004100
C	4.88059600	-1.45361100	2.70353800
C	4.12590700	0.08566800	-1.70865500

C	-1.99140700	-3.60602400	-1.72667200
C	3.88901800	-1.40521100	1.70284700
C	-2.66076900	0.97597400	2.43083800
C	0.46993000	-2.79452400	2.42868600
C	1.35253000	2.48623300	-2.42350000
C	-1.02595000	-3.04459400	2.53751300
C	-2.12742500	2.39488800	2.54935800
C	0.01898100	3.20682900	-2.54086000
C	-2.55869500	3.28255500	3.55638900
C	-1.58323900	-3.86619400	3.53864600
C	-0.23806700	4.16198100	-3.54564200
C	-1.18197800	4.94391100	2.71686400
C	-3.70614100	-3.50491900	2.68889000
C	-2.36738800	4.50934200	-2.70592800
C	-3.16581600	-2.67080100	1.68931400
C	-0.73158100	4.06482600	1.71132100
C	-2.13045700	3.54775400	-1.70285800
H	1.62128200	-5.62190000	2.49391500
H	-5.68834700	1.39526300	2.49183100
H	3.35333800	4.79676400	-2.48407900
H	-7.82451200	1.50539000	1.22430400
H	2.59860800	-7.52698200	1.23049300
H	4.88997100	6.28533500	-1.21649400
H	3.03408400	-7.36773600	-1.20288900
H	-7.89887300	1.05927300	-1.21118000
H	5.24214300	5.99597500	1.21825500
H	-5.83896500	0.49300300	-2.48300900
H	2.50327300	-5.29957700	-2.47626100
H	4.06751900	4.21115900	2.48924200
H	1.47566300	-3.22862900	-3.16170900
H	-3.52317500	0.35746500	-3.16584600
H	2.42212200	2.57229600	3.17158500
H	-1.84178300	0.36414700	-2.62248000
H	0.62112900	-1.77707800	-2.62918600
H	1.15546100	1.46707500	2.62512400
H	3.58099400	-2.64508800	-4.29143900
H	-4.07112900	-1.75193200	-4.30752800
H	4.23903500	1.34793600	4.29587300
H	6.00994200	0.36963200	-2.77288100
H	-2.68353900	-5.37276600	-2.80494800
H	5.58672400	-2.27536800	2.76284500
H	-1.40457600	-4.14379000	-0.99161600
H	4.29152500	0.86457000	-0.97399100
H	3.80006800	-2.19288500	0.96424000
H	0.68730900	-1.74099900	2.63235900
H	-1.85746400	0.25838500	2.62748400
H	1.21647900	1.41738900	-2.61860600
H	-3.44771600	0.80532600	3.17020800
H	1.00747800	-3.39352500	3.16844400
H	2.05766000	2.87313600	-3.16393600
H	-0.96312000	-4.35136800	4.28689200
H	-3.28933600	2.98445400	4.30277000
H	0.50887800	4.41831900	-4.29142500
H	-4.77110900	-3.70483500	2.74616800
H	-0.82113500	5.96525000	2.78074200
H	-3.31012800	5.04294100	-2.76872000

H	-0.00551800	4.38288700	0.97269800
H	-3.80175400	-2.19822400	0.95033000
H	-2.88844500	3.30786900	-0.96679300
N	-1.42507700	4.81141100	-3.63152400
N	4.99680000	-0.47279200	3.63115000
N	4.87802600	-1.15650000	-3.63382300
N	-2.91687400	-4.09665600	3.61779900
N	-3.43427800	-3.62374100	-3.65865500
N	-2.08916100	4.55138300	3.64369700