Hexacoordinate Planar Main Group Atoms Centered in hexagonal hydrocopper Complexes $\text{Cu}_6\text{H}_6\text{X}$ (X=Si,P,As)

Si-Dian Li*, Guang-Ming Ren, and Chang-Qing Miao

Institute of Materials sciences and Department of Chemistry, Xinzhou Teachers' University, Xinzhou 034000, Shanxi, P. R. China.

Supporting Information

Optimized Cartesian coordinates (x,y,z) of $\text{Cu}_6\text{H}_6\text{X}$ complexes

in angstroms at B3LYP/6-311+G(d,p) level

1. D_{6h} $\text{Cu}_6\text{H}_6\text{Si}$

Atomic Number	X	Y	Z
29	0.000000	2.461463	0.000000
29	2.131689	1.230731	0.000000
29	2.131689	-1.230731	0.000000
29	0.000000	-2.461463	0.000000
29	-2.131689	-1.230731	0.000000
29	-2.131689	1.230731	0.000000
1	1.576373	2.730358	0.000000
1	3.152746	0.000000	0.000000
1	-1.576373	2.730358	0.000000
1	-1.576373	-2.730358	0.000000
1	-3.152746	0.000000	0.000000
1	1.576373	-2.730358	0.000000
14	0.000000	0.000000	0.000000

2. C_{6v} Cu₆H₆Si

Atomic Number	X	Y	Z
29	0.000000	2.460587	-0.009323
29	-2.130931	1.230293	-0.009323
29	-2.130931	-1.230293	-0.009323
29	0.000000	-2.460587	-0.009323
29	2.130931	-1.230293	-0.009323
29	2.130931	1.230293	-0.009323
1	-1.577692	2.732643	0.013581
1	-3.155384	0.000000	0.013581
1	1.577692	2.732643	0.013581
1	1.577692	-2.732643	0.013581
1	3.155384	0.000000	0.013581
1	-1.577692	-2.732643	0.013581
14	0.000000	0.000000	0.110053

3. C_{2v} Cu₆H₆Si

Atomic Number	X	Y	Z
29	0.000000	2.452801	-0.023204
29	-2.123314	1.226434	-0.027324
29	-2.123314	-1.226434	-0.027324
29	0.000000	-2.452801	-0.023204
29	2.123314	-1.226434	-0.027324
29	2.123314	1.226434	-0.027324
1	-1.575762	2.729510	0.035475
1	-3.150132	0.000000	0.030680
1	1.575762	2.729510	0.035475
1	1.575762	-2.729510	0.035475
1	3.150132	0.000000	0.030680

1	-1.575762	-2.729510	0.035475
14	0.000000	0.000000	0.308007

4. D_{6h} $Cu_6H_6Si^+$

Atomic Number	X	Y	Z
29	0.000000	2.525352	0.000000
29	2.187019	1.262676	0.000000
29	2.187019	-1.262676	0.000000
29	0.000000	-2.525352	0.000000
29	-2.187019	-1.262676	0.000000
29	-2.187019	1.262676	0.000000
1	1.579761	2.736227	0.000000
1	3.159522	0.000000	0.000000
1	-1.579761	2.736227	0.000000
1	-1.579761	-2.736227	0.000000
1	-3.159522	0.000000	0.000000
1	1.579761	-2.736227	0.000000
14	0.000000	0.000000	0.000000

5. D_{6h} $Cu_6H_6P^+$

Atomic Number	X	Y	Z
29	0.000000	2.482996	0.000000
29	2.150338	1.241498	0.000000
29	2.150338	-1.241498	0.000000
29	0.000000	-2.482996	0.000000
29	-2.150338	-1.241498	0.000000
29	-2.150338	1.241498	0.000000
1	1.566783	2.713748	0.000000
1	3.133566	0.000000	0.000000

1	-1.566783	2.713748	0.000000
1	-1.566783	-2.713748	0.000000
1	-3.133566	0.000000	0.000000
1	1.566783	-2.713748	0.000000
15	0.000000	0.000000	0.000000

6. C_{6v} Cu_6H_6Ge

Atomic Number	X	Y	Z
29	1.231009	2.132170	-0.114639
29	-1.231009	2.132170	-0.114639
29	-2.462018	0.000000	-0.114639
29	-1.231009	-2.132170	-0.114639
29	1.231009	-2.132170	-0.114639
29	2.462018	0.000000	-0.114639
1	0.000000	3.156318	-0.005265
1	-2.733451	1.578159	-0.005265
1	2.733451	1.578159	-0.005265
1	0.000000	-3.156318	-0.005265
1	2.733451	-1.578159	-0.005265
1	-2.733451	-1.578159	-0.005265
32	0.000000	0.000000	0.624336

7. D_{6h} $Cu_6H_6As^+$

Atomic Number	X	Y	Z
29	0.000000	2.541240	0.000000
29	2.200778	1.270620	0.000000
29	2.200778	-1.270620	0.000000
29	0.000000	-2.541240	0.000000
29	-2.200778	-1.270620	0.000000

29	-2.200778	1.270620	0.000000
1	1.575585	2.728993	0.000000
1	3.151170	0.000000	0.000000
1	-1.575585	2.728993	0.000000
1	-1.575585	-2.728993	0.000000
1	-3.151170	0.000000	0.000000
1	1.575585	-2.728993	0.000000
33	0.000000	0.000000	0.000000

8. Calculated Harmonic vibrational frequencies at B3LYP/6-311+G(d,p)

ν /cm ⁻¹	Cu ₆ H ₆ Si (D _{6h})	Cu ₆ H ₆ Si (C _{6v})	Cu ₆ H ₆ Si (C _{2v})	Cu ₆ H ₆ Si ⁺ (D _{6h})	Cu ₆ H ₆ P ⁺ (D _{6h})	Cu ₆ H ₆ Ge (C _{6v})	Cu ₆ H ₆ As ⁺ (D _{6h})
ν_1	-29	-28	42	33	19	43	35
ν_2	42	43	44	42	32	43	46
ν_3	46	46	47	63	74	62	49
ν_4	80	82	81	84	74	78	89
ν_5	80	89	85	84	86	79	89
ν_6	90	89	86	98	96	79	90
ν_7	116	115	114	110	102	116	116
ν_8	118	133	142	142	156	127	137
ν_9	121	137	147	158	171	127	137
ν_{10}	161	161	163	158	171	158	152
ν_{11}	170	183	220	200	198	158	183
ν_{12}	170	185	222	200	198	158	183
ν_{13}	219	219	228	201	219	214	195
ν_{14}	220	220	230	220	219	214	199
ν_{15}	227	228	233	233	220	223	200
ν_{16}	254	254	288	234	227	293	246
ν_{17}	255	255	290	347	348	377	346
ν_{18}	317	323	316	384	373	377	390
ν_{19}	358	366	366	477	452	445	442
ν_{20}	361	368	370	507	471	445	482
ν_{21}	543	547	547	574	587	555	591
ν_{22}	1389	1383	1376	1377	1405	1334	1354
ν_{23}	1392	1385	1378	1382	1424	1334	1376
ν_{24}	1409	1405	1413	1385	1426	1402	1379
ν_{25}	1413	1409	1415	1388	1431	1402	1389
ν_{26}	1413	1410	1419	1390	1432	1410	1392
ν_{27}	1430	1426	1430	1416	1455	1416	1416
ν_{28}	1479	1469	1464	1547	1580	1435	1589
ν_{29}	1534	1523	1519	1598	1630	1493	1637
ν_{30}	1541	1530	1523	1601	1637	1493	1642
ν_{31}	1628	1619	1615	1688	1730	1590	1732
ν_{32}	1634	1624	1618	1690	1736	1590	1735
ν_{33}	1653	1642	1636	1719	1765	1608	1771