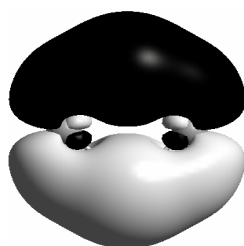
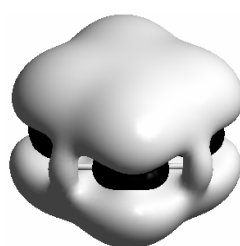


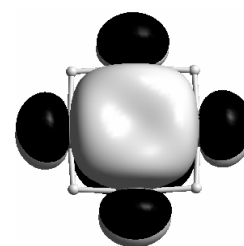
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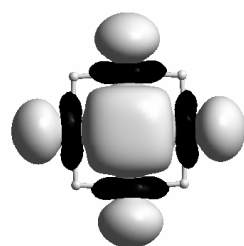
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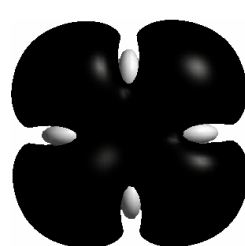
HOMO-11



HOMO-17

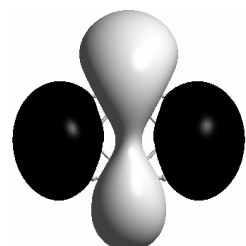


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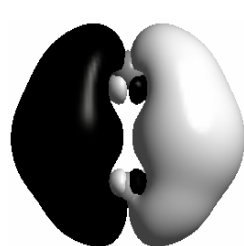


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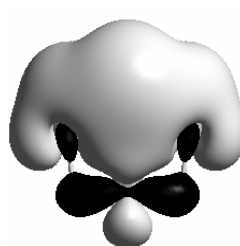
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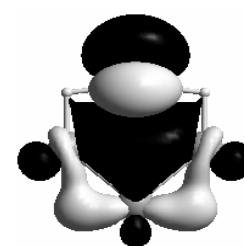
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HOMO

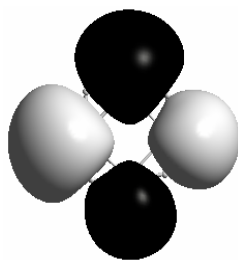


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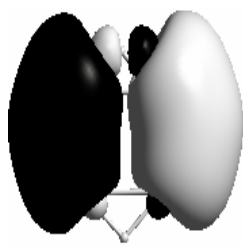


HOMO-20

6



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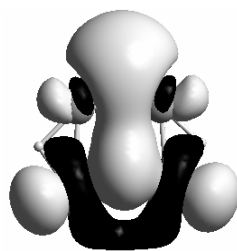
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HOMO-12

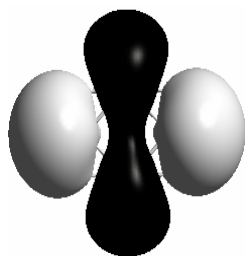


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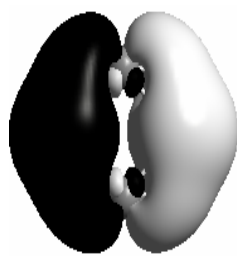


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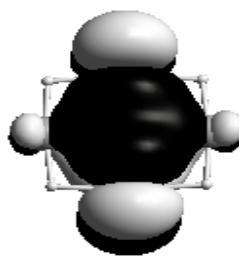
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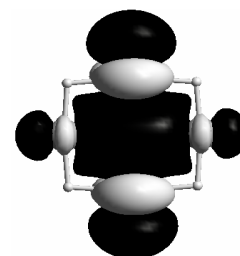
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HOMO

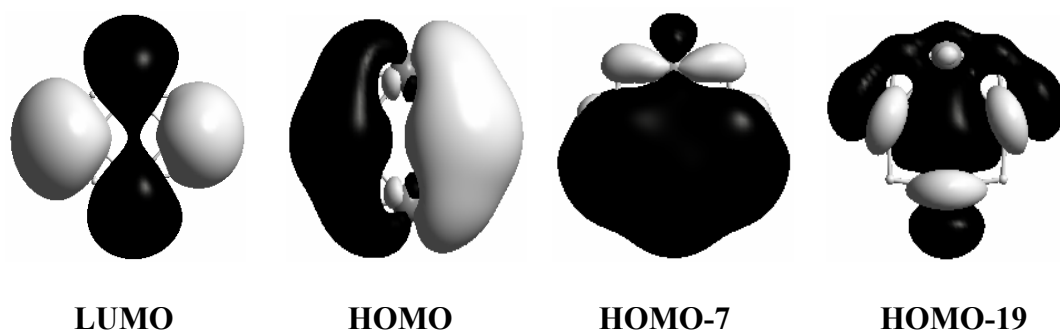


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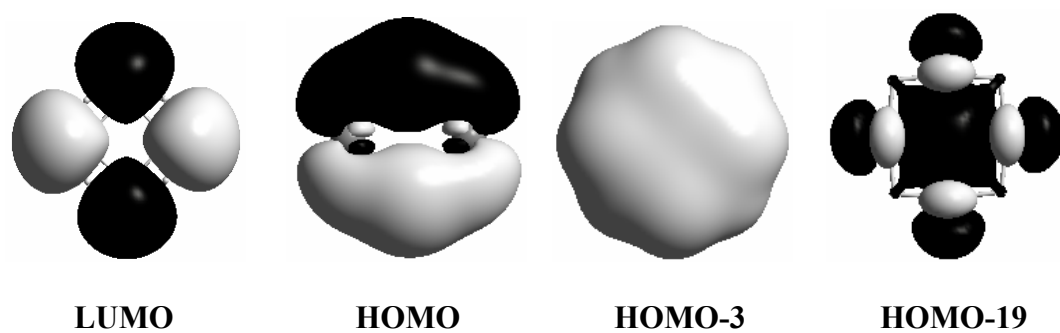


HOMO-19

8

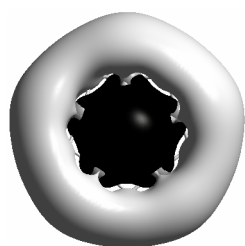


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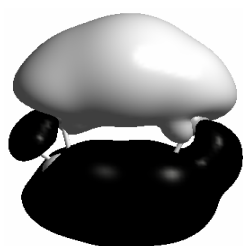


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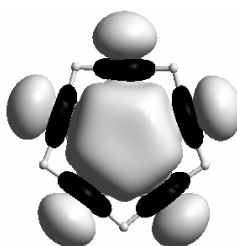
Figure S1



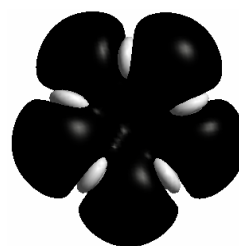
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HOMO

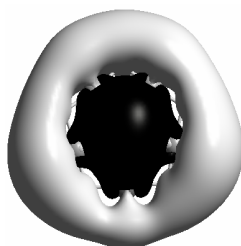


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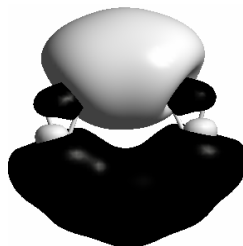


HOMO-29

11



LUMO

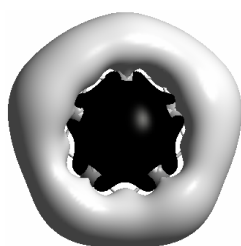


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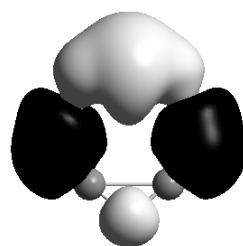


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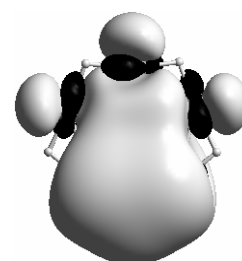
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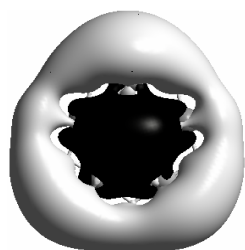


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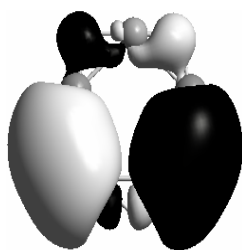


HOMO-15

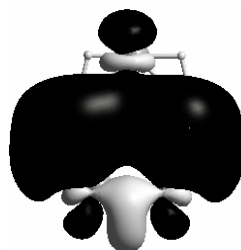
13



LUMO



HOMO

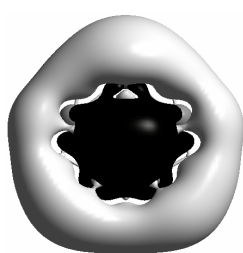


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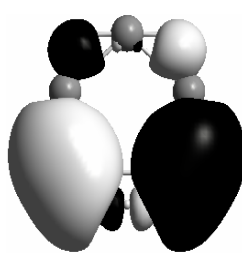


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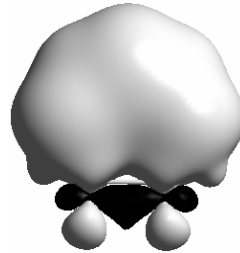
14



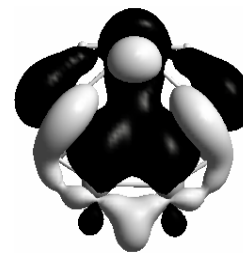
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HOMO

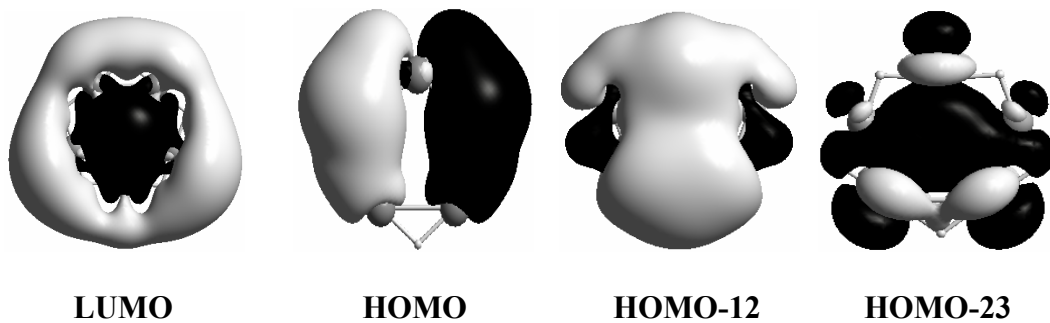


HOMO-11

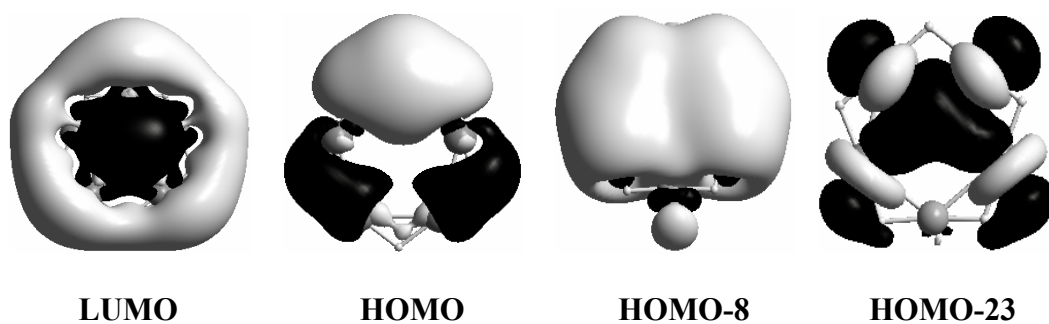


HOMO-21

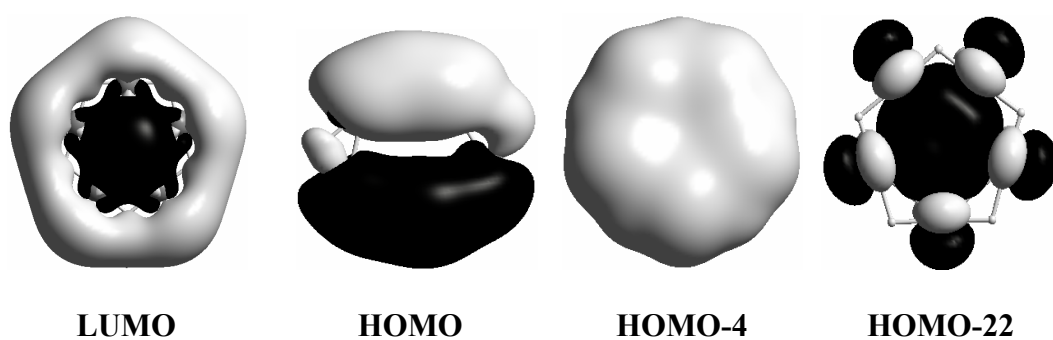
15



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18

Figure S2

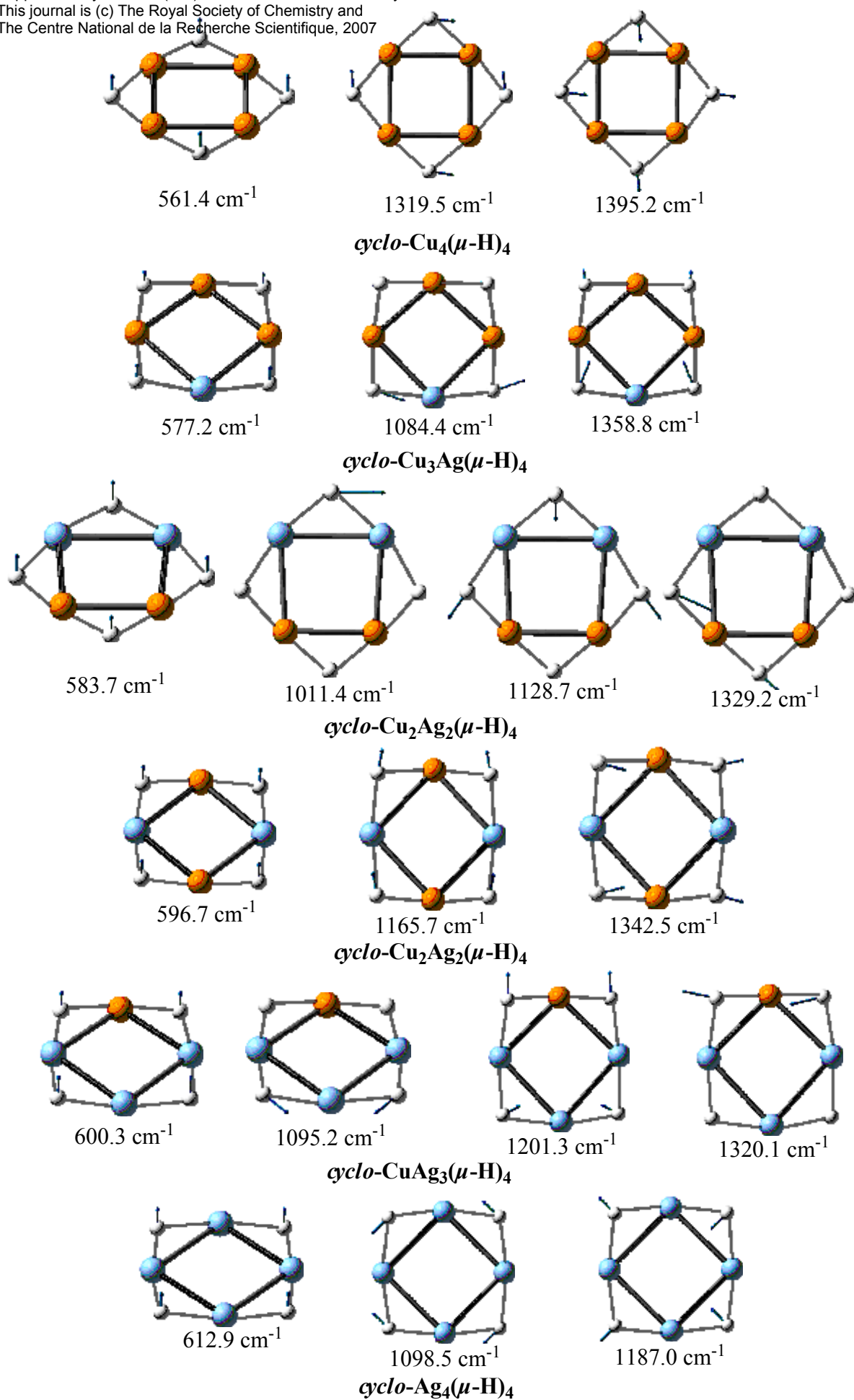


Figure S3

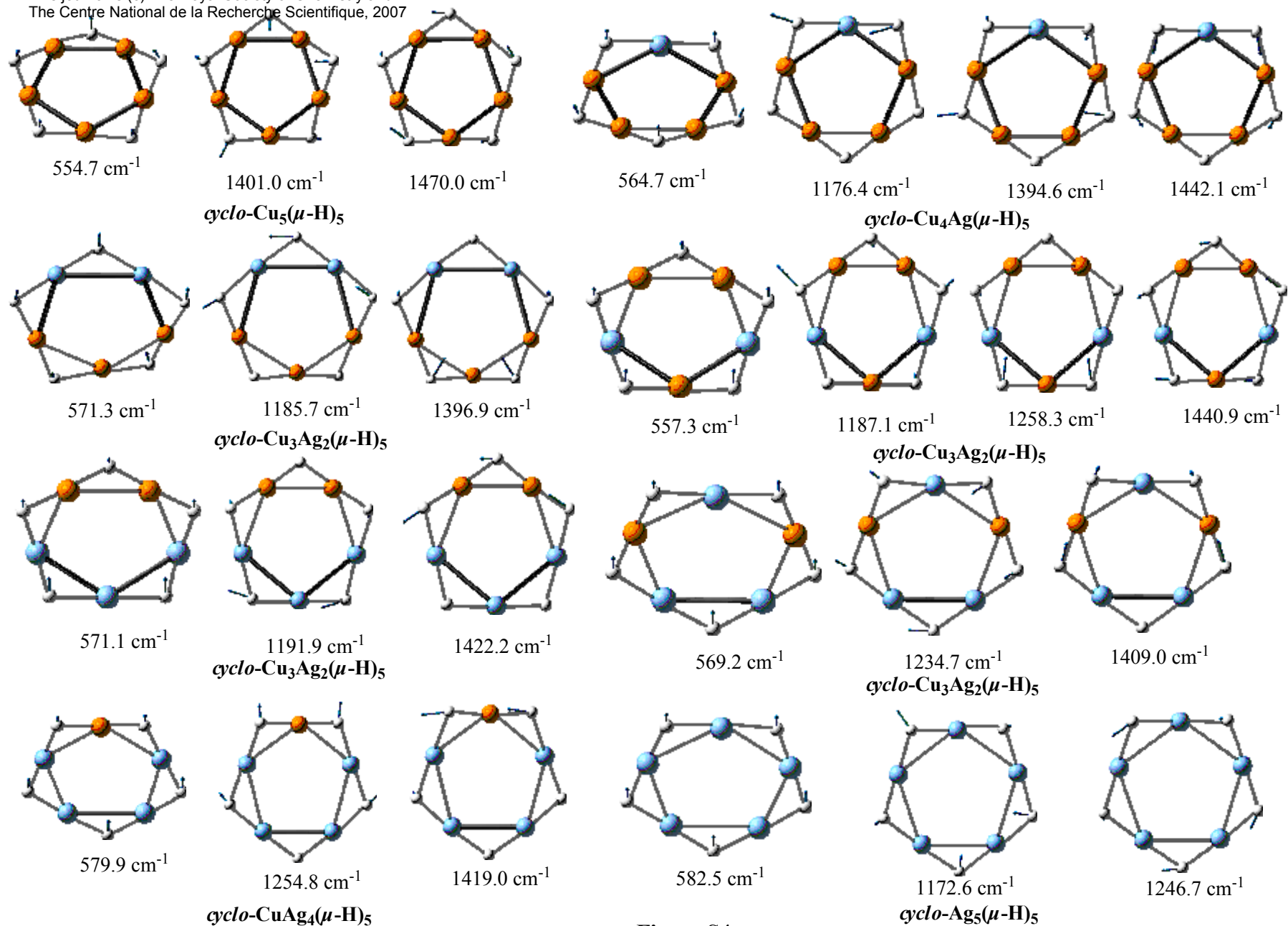


Figure S4

Table S1 The most intense unscaled vibrational frequencies and the IR intensities computed at the b3lyp/6-31G(d,p)∪lanl2dz(Ag) level.

Species	Frequency (cm ⁻¹)	Intensity (KMmol ⁻¹)
1	559	0.33
	1035	1.00
	1294	0.57
2	546	0.25
	722	0.38
	905	1.00
	1251	0.60
3	546	0.25
	722	0.38
	905	1.00
	1251	0.60
4	536	0.26
	846	1.00
	1075	0.33
5	561	0.42
	1320	0.56
	1395	1.00
6	577	0.31
	1084	0.42
7	1359	1.00
	584	0.43
	1011	0.71
8	1129	0.92
	1329	1.00
	597	0.23
	1168	1.00
9	1342	0.88
	600	0.42
	1095	0.99
10	1201	0.94
	1320	1.00
	613	0.31
	1100	1.00
11	1187	0.56
	555	0.39
	1404	0.44
12	1470	1.00
	565	0.35
	1395	0.50
	1442	1.00
13	571	0.49
	1186	1.00
	1397	0.84
	1419	0.67

14	557	0.33
	1258	0.37
	1387	0.41
	1441	1.00
15	571	0.47
	1192	0.91
	1267	0.58
	1442	1.00
16	569	0.31
	1235	1.00
	1409	0.89
17	580	0.45
	1191	0.55
	1255	1.00
	1419	0.76
18	583	0.26
	1173	0.24
	1249	1.00