

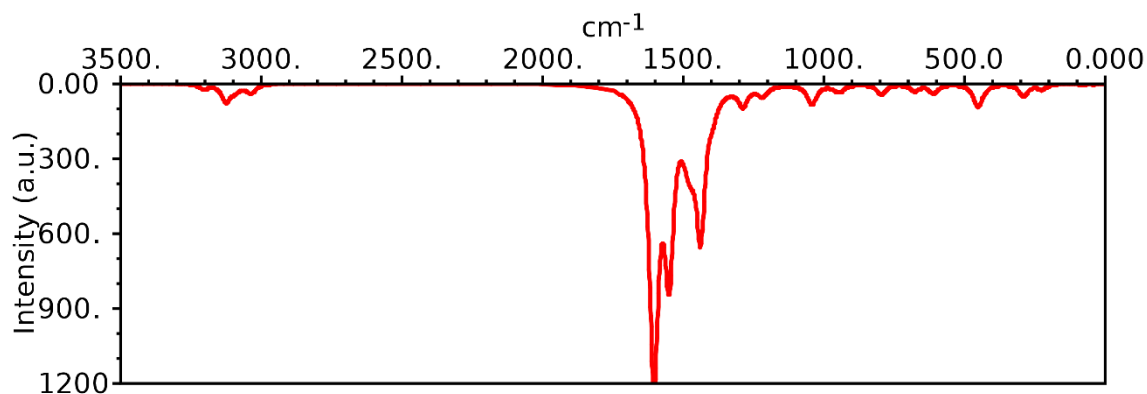
SUPPLEMENTAL INFORMATION

SI1. Vibrational Levels of the neutral D_{2h} -symmetry [Cu(acac)₂]

Harmonic frequencies calculated at B3LYP/aug-cc-pvtz level and the option "SuperFineGrid" for numerical integrations. The infrared spectrum is also showed.

Harmonic frequencies (cm⁻¹)

Frequencies --	13.1578	41.8791	79.1772
Frequencies --	82.6699	85.6819	89.9073
Frequencies --	90.6232	108.3022	139.2796
Frequencies --	146.3377	161.1090	161.7266
Frequencies --	191.9810	204.5761	227.2231
Frequencies --	256.1251	261.7810	292.8149
Frequencies --	330.9174	411.4235	436.0072
Frequencies --	445.0441	455.5132	570.6236
Frequencies --	574.7841	575.2294	612.6971
Frequencies --	677.4795	678.9972	679.3558
Frequencies --	681.0317	797.9653	798.2347
Frequencies --	940.8968	945.8533	962.6076
Frequencies --	964.2479	1037.4266	1039.3451
Frequencies --	1044.2738	1047.2723	1047.4585
Frequencies --	1047.5858	1060.1181	1060.2555
Frequencies --	1216.8805	1220.2722	1290.3481
Frequencies --	1292.4938	1395.3715	1395.4982
Frequencies --	1396.5614	1396.9727	1416.1803
Frequencies --	1441.0026	1473.4381	1473.6061
Frequencies --	1474.1795	1474.4239	1477.6628
Frequencies --	1478.9862	1490.6832	1496.3362
Frequencies --	1550.8165	1552.4951	1606.8405
Frequencies --	1626.4244	3039.2713	3039.2893
Frequencies --	3039.3289	3039.4110	3094.7001
Frequencies --	3094.7045	3094.8039	3094.8319
Frequencies --	3127.8234	3127.9365	3128.0593
Frequencies --	3128.1237	3206.2102	3206.3355

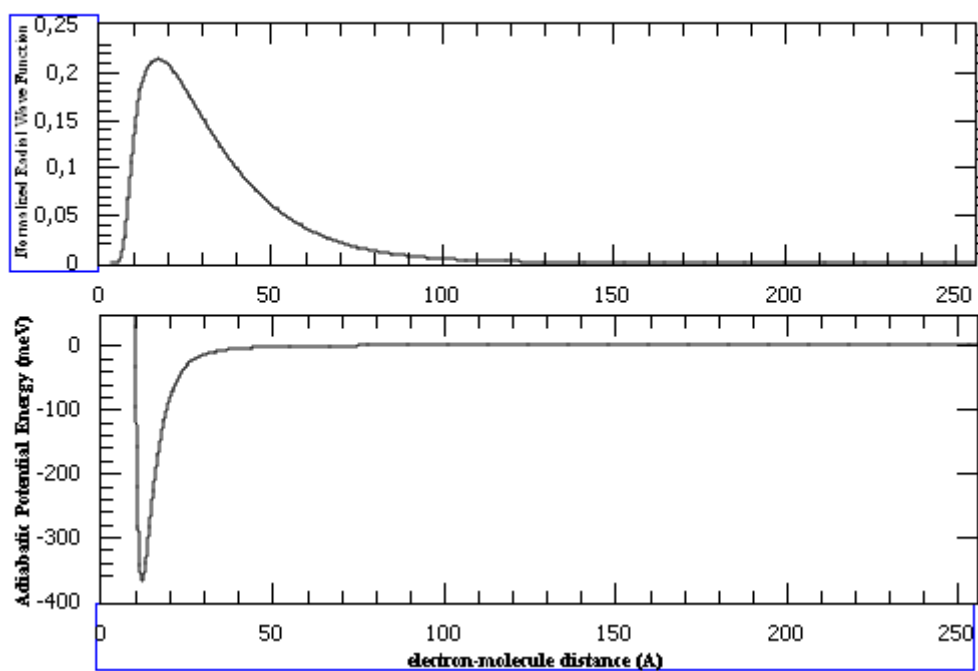


SI2. Excited states of the neutral D_{2h} -symmetry [Cu(acac)₂]

Calculations at TDDFT/B3LYP/aug-cc-pvtz level. The first four LUMO present the π^* , π^* , non bonding s-orbital on Cu and σ^* , respectively.

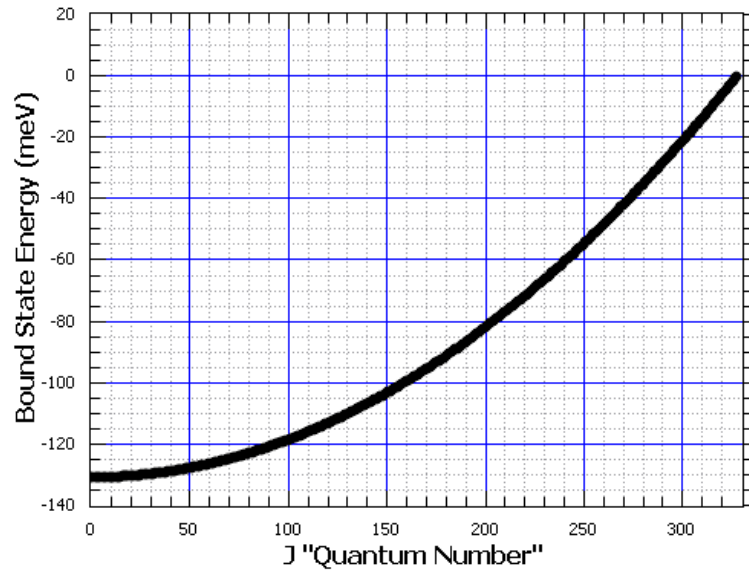
			(eV)		(nm)	oscillator strength (a.u.)
Excited State	1:	2.0073	eV	617.67	nm	f=0.0000
Excited State	2:	2.1977	eV	564.16	nm	f=0.0000
Excited State	3:	2.5043	eV	495.08	nm	f=0.0000
Excited State	4:	2.5203	eV	491.94	nm	f=0.0000
Excited State	5:	3.0110	eV	411.78	nm	f=0.0000
Excited State	6:	3.1315	eV	395.92	nm	f=0.0000
Excited State	7:	3.1541	eV	393.10	nm	f=0.0000
Excited State	8:	3.3244	eV	372.95	nm	f=0.0000
Excited State	9:	3.5942	eV	344.95	nm	f=0.2421
Excited State	10:	3.6342	eV	341.16	nm	f=0.0000
Excited State	11:	3.7199	eV	333.30	nm	f=0.0002
Excited State	12:	4.1023	eV	302.23	nm	f=0.0105
Excited State	13:	4.3061	eV	287.93	nm	f=0.0000
Excited State	14:	4.4664	eV	277.59	nm	f=0.0000
Excited State	15:	4.4820	eV	276.62	nm	f=0.0011
Excited State	16:	4.5152	eV	274.59	nm	f=0.0041
Excited State	17:	4.5404	eV	273.07	nm	f=0.0000
Excited State	18:	4.5513	eV	272.42	nm	f=0.0020
Excited State	19:	4.5603	eV	271.88	nm	f=0.0000
Excited State	20:	4.7743	eV	259.69	nm	f=0.0000
Excited State	21:	5.0586	eV	245.10	nm	f=0.0000
Excited State	22:	5.0720	eV	244.45	nm	f=0.0008
Excited State	23:	5.0791	eV	244.11	nm	f=0.0000
Excited State	24:	5.1522	eV	240.64	nm	f=0.0000
Excited State	25:	5.1585	eV	240.35	nm	f=0.0000
Excited State	26:	5.1682	eV	239.90	nm	f=0.0000
Excited State	27:	5.1758	eV	239.55	nm	f=0.5647
Excited State	28:	5.2216	eV	237.44	nm	f=0.0000
Excited State	29:	5.3346	eV	232.42	nm	f=0.0012
Excited State	30:	5.3389	eV	232.23	nm	f=0.0000

SI3. Adiabatic Potential Curve and Normalized Radial wave function



SI4 : (a) multipole bound ($J, k=0$) states and (b) Population of accessible bound « j » states following the Boltzmann distribution.

(a) Multipole bound ($J, k=0$) states. The last bound « J » state (i.e. $E < 0$) is obtained for $J=328$.



(b) Population of accessible bound « j » states. For each « j » state, the population of accessible bound states is integrated over all possible « k » states.

