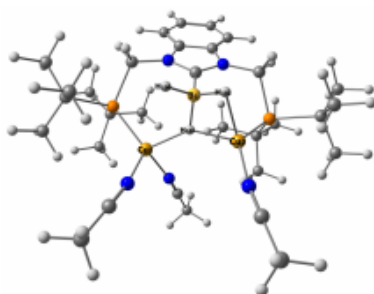


$\nu_{\text{experimental}}(\text{cm}^{-1})$	$\nu_{\text{experimental}}(\text{cm}^{-1})$	Assignment	$\nu_{\text{experimental}}(\text{cm}^{-1})$	$\nu_{\text{experimental}}(\text{cm}^{-1})$	Assignment	Assignment
n.d.	1901	B-H101	n.d.	2213	B-H102	B-H102
2277	2264; 2267; 2271	C $\equiv$ N	2277	2264; 2267; 2271	C $\equiv$ N	C $\equiv$ N
2317	2495	B-H100	2317	2495	B-H100	B-H100
2423			2423			

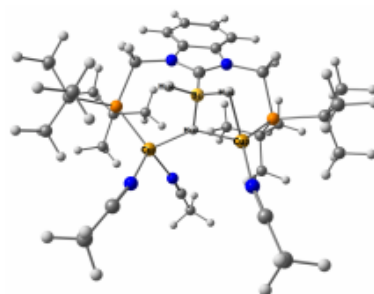
\*RI-BP86-D3 / def2-TZVP

Scale Factor: 0.9953 (*J. Phys. Chem. A*, 2015, 119, 9, 1701–1714)

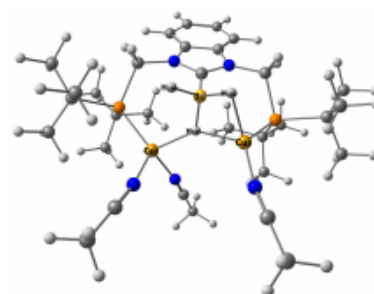
## Vibrational modes animations and their frequency values



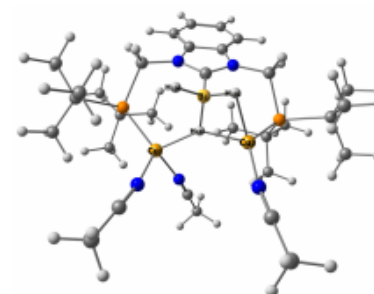
2495



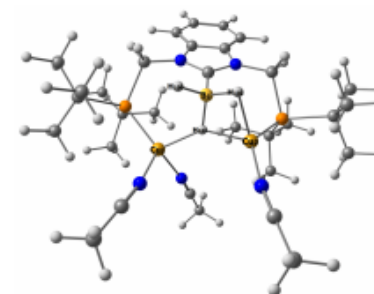
2271



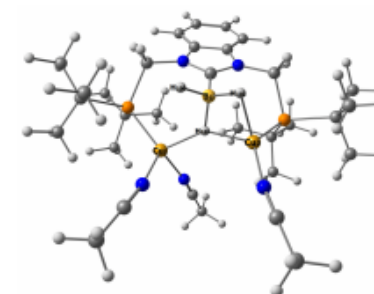
2267



2264



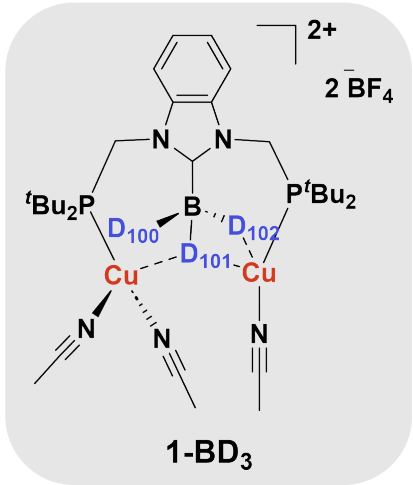
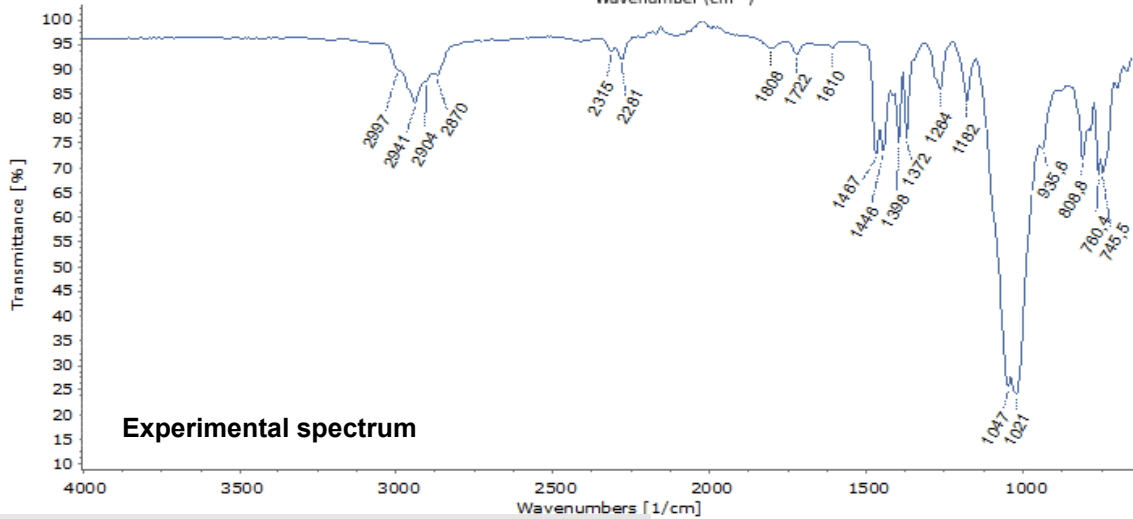
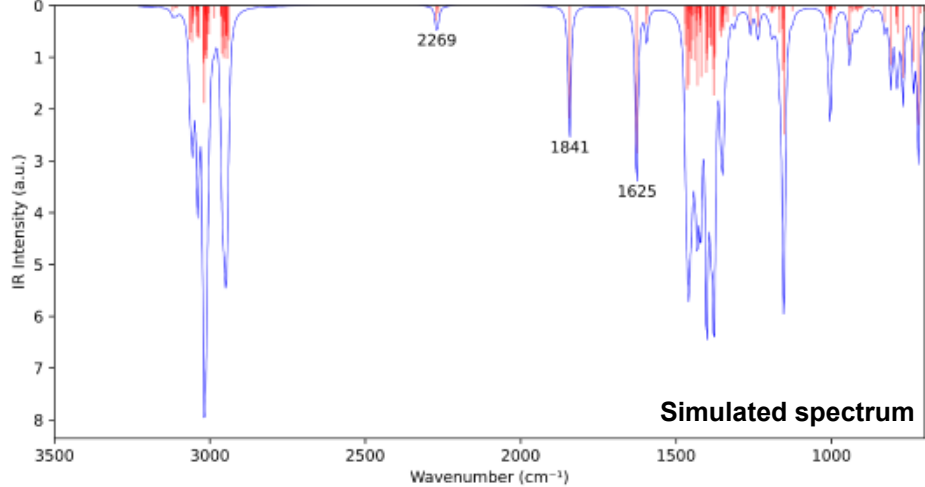
2213



1901

# Experimental and theoretical frequencies of 1-BD<sub>3</sub>

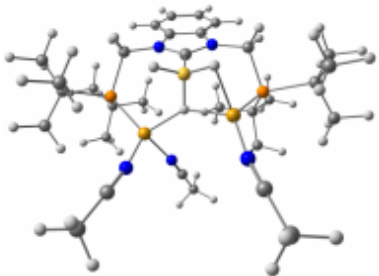
Vibrational modes associated to the acetonitrile ligands are the same than 1



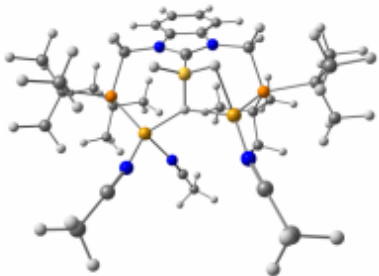
$\nu_{\text{exp}}(\text{cm}^{-1})$	$\nu_{\text{calc}}(\text{cm}^{-1})$	Assignment	$\nu_{\text{exp}}(\text{cm}^{-1})$	$\nu_{\text{calc}}(\text{cm}^{-1})$	Assignment	Assignment
n.d.	1375; 1376; 1386; 1387	B-D101	1722	1625	B-D102	
1808	1841	B-D100	2315	2264; 2268; 2272	C $\equiv$ N	

\*RI-BP86-D3 / def2-TZVP  
Scale Factor: 0.9953 (*J. Phys. Chem. A*, **2015**, 119, 9, 1701–1714)

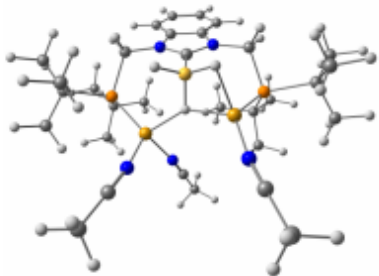
## Vibrational modes animations and their frequency values



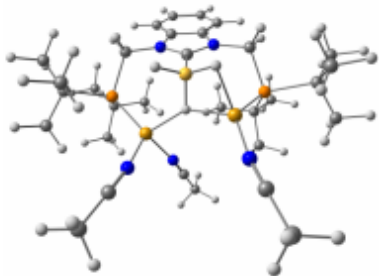
1841



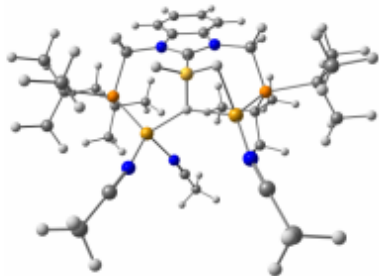
1625



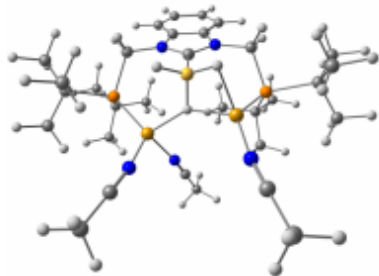
1387



1386

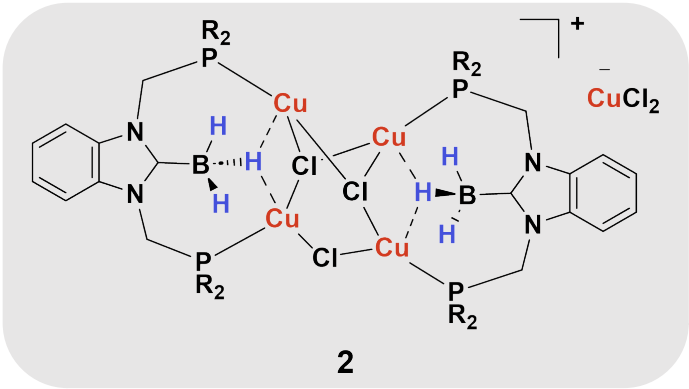
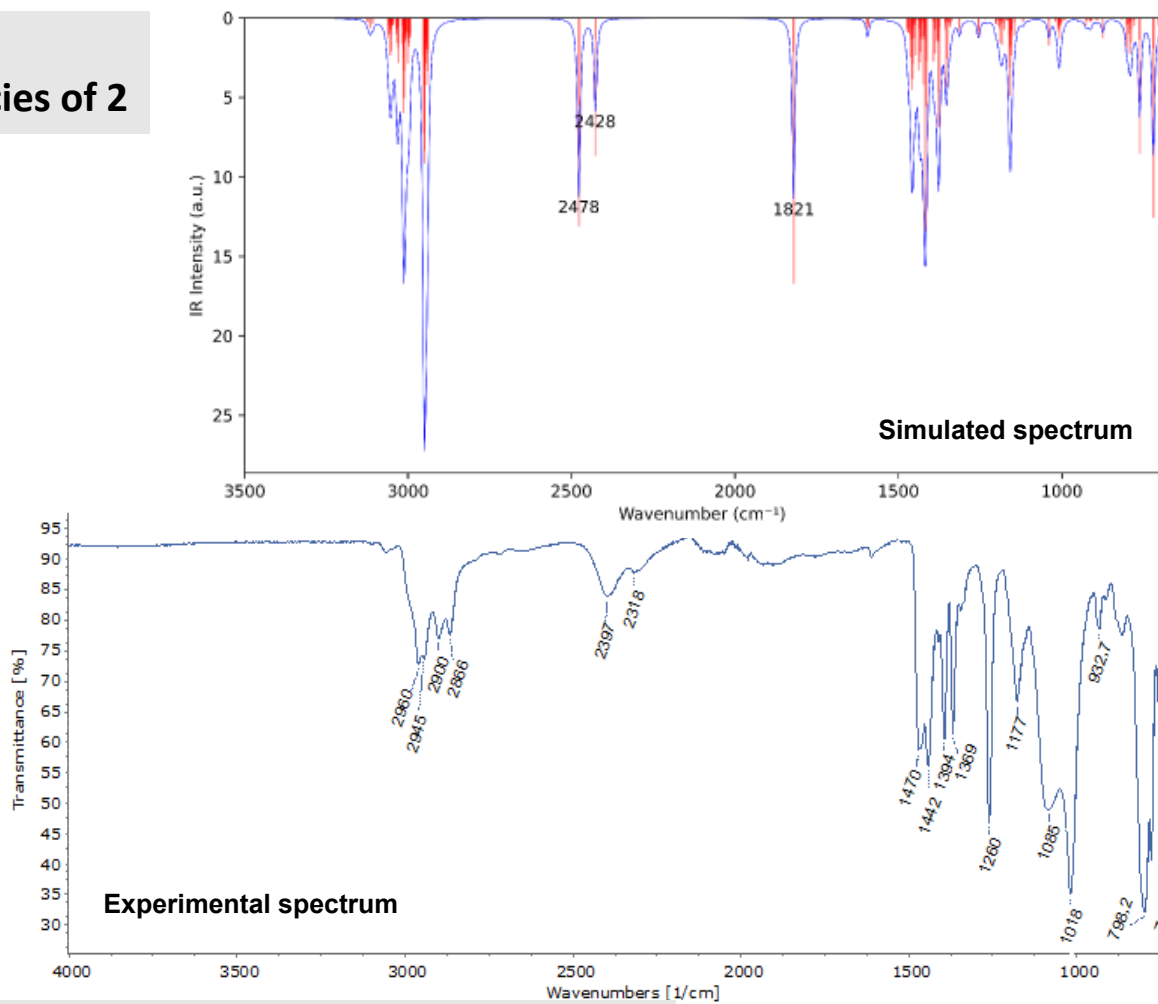


1376



1375

# Experimental and theoretical frequencies of 2

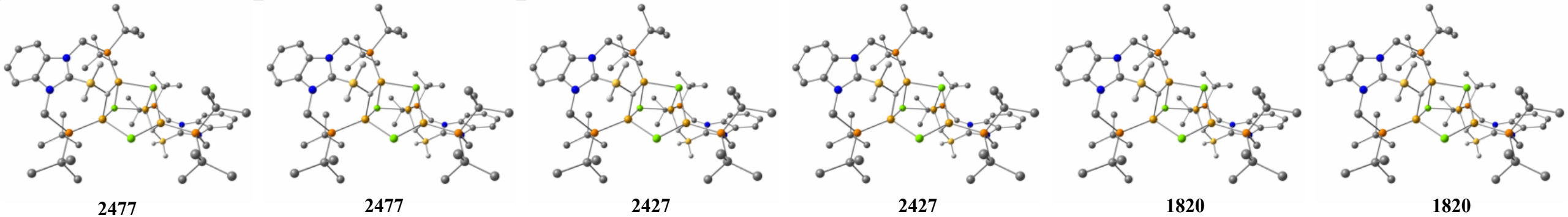


$\nu_{\text{B-H}_{\text{bridging}}}$ (cm <sup>-1</sup> )	$\nu_{\text{B-H}_{\text{terminals}}}$ (cm <sup>-1</sup> )	Assignment	$\nu_{\text{B-H}_{\text{bridging}}}$ (cm <sup>-1</sup> )	$\nu_{\text{B-H}_{\text{terminals}}}$ (cm <sup>-1</sup> )	Assignment
n.d.	1820 (x2)	B-H <sub>bridging</sub>	n.d.	1820 (x2)	B-H <sub>bridging</sub>
2318	2427 (x2)	B-H <sub>terminals</sub> (sym.)	2398	2427 (x2)	B-H <sub>terminals</sub> (sym.)
2397	2477 (x2)	B-H <sub>terminals</sub> (asym.)	2397	2477 (x2)	B-H <sub>terminals</sub> (asym.)

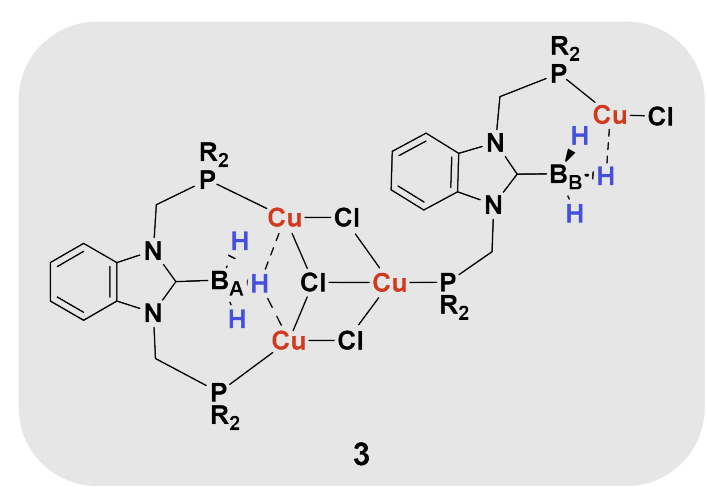
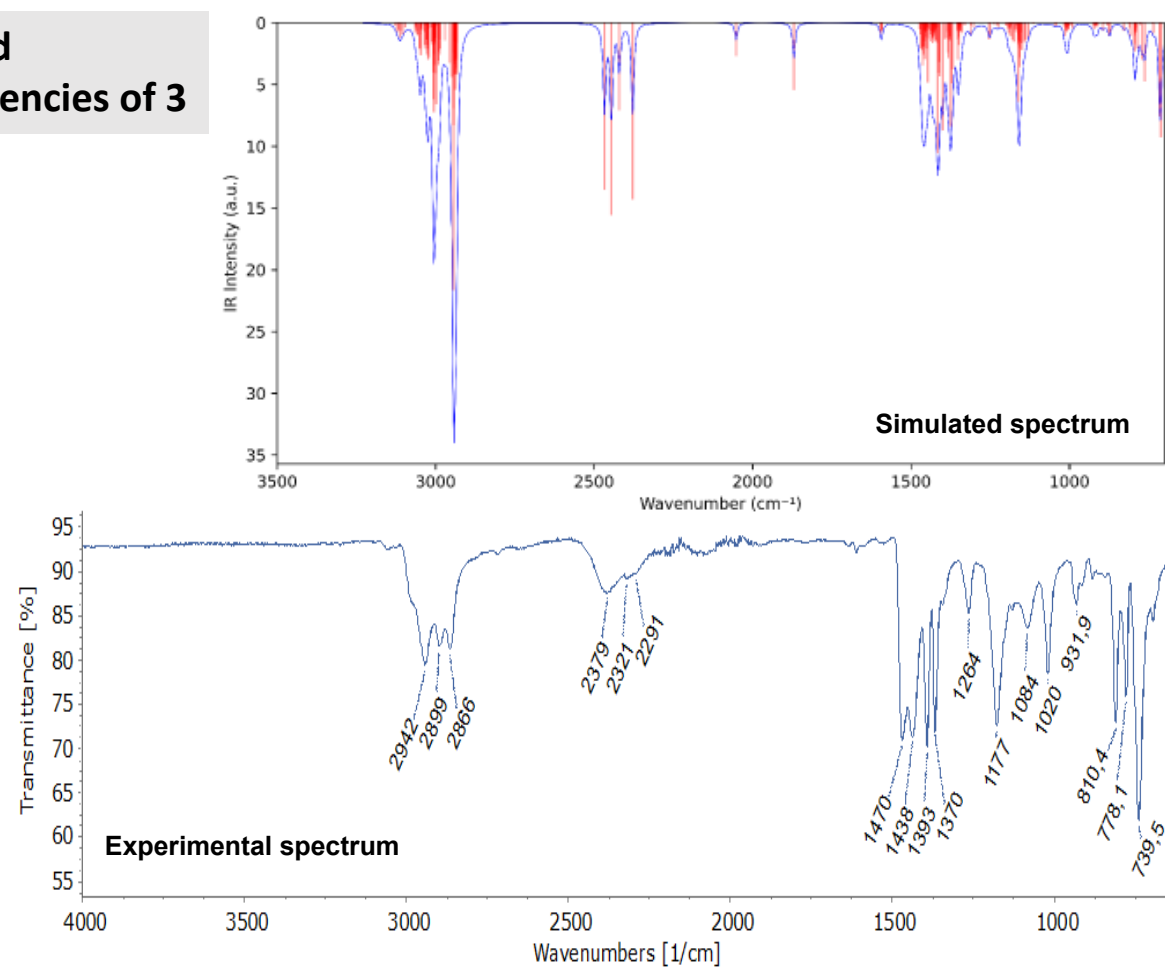
\*RI-BP86-D3 / def2-TZVP  
Scale Factor: 0.9953 (*J. Phys. Chem. A*, **2015**, 119, 9, 1701–1714)

## Vibrational modes animations and their frequency values

Hydrogens bonded to carbon atoms were hidden for clarity of the animations



Experimental and theoretical frequencies of 3



Assignment		
n.d.	1869	$\mu^2$ - B-H <sub>bridging</sub>
	2051	$\mu^1$ - B-H
	2378	B <sub>B</sub> -H <sub>terminals</sub> (sym.)
	2420	B <sub>A</sub> -H <sub>terminals</sub> (sym.)
	2445	B <sub>B</sub> -H <sub>terminals</sub> (asym.)
	2467	B <sub>A</sub> -H <sub>terminals</sub> (asym.)

Vibrational modes animations and their frequency values

Hydrogens bonded to carbon atoms were hidden for clarity of the animations

\*RI-BP86-D3 / def2-TZVP  
Scale Factor: 0.9953 (*J. Phys. Chem. A*, 2015, 119, 9, 1701–1714)

