ELECTRONIC SUPPLEMENTARY INFORMATION

X-ray Raman Optical Activity of Molecules

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1) Raman vs chiral contribution

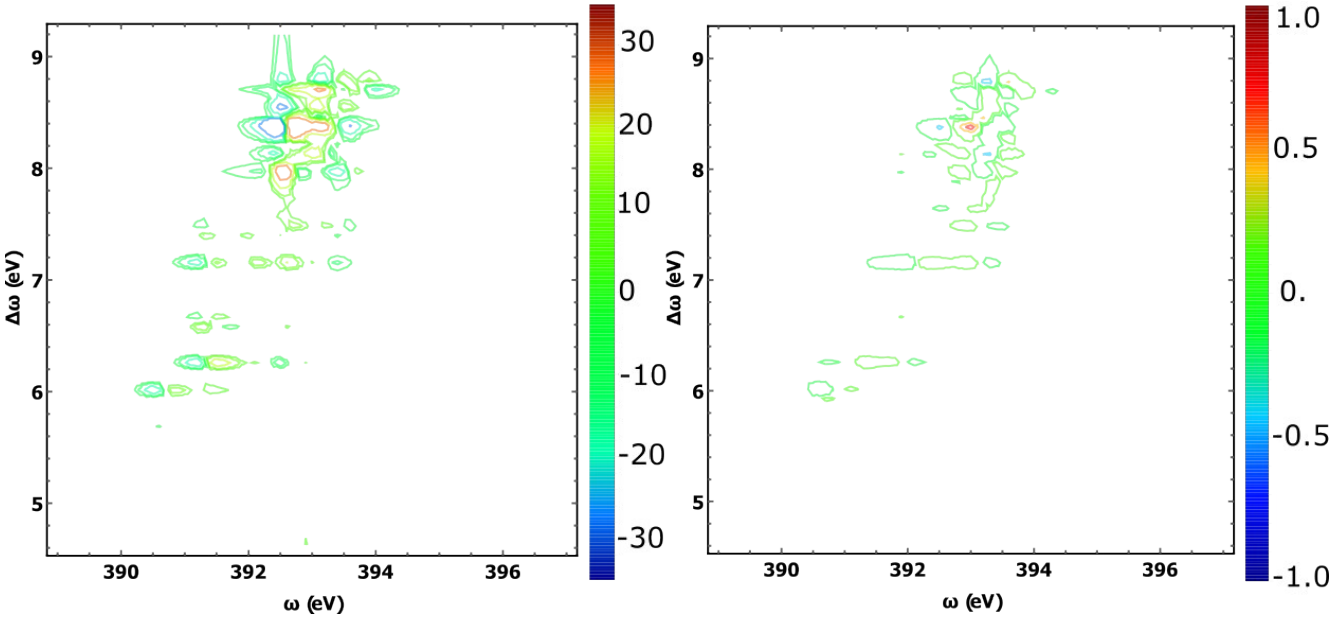
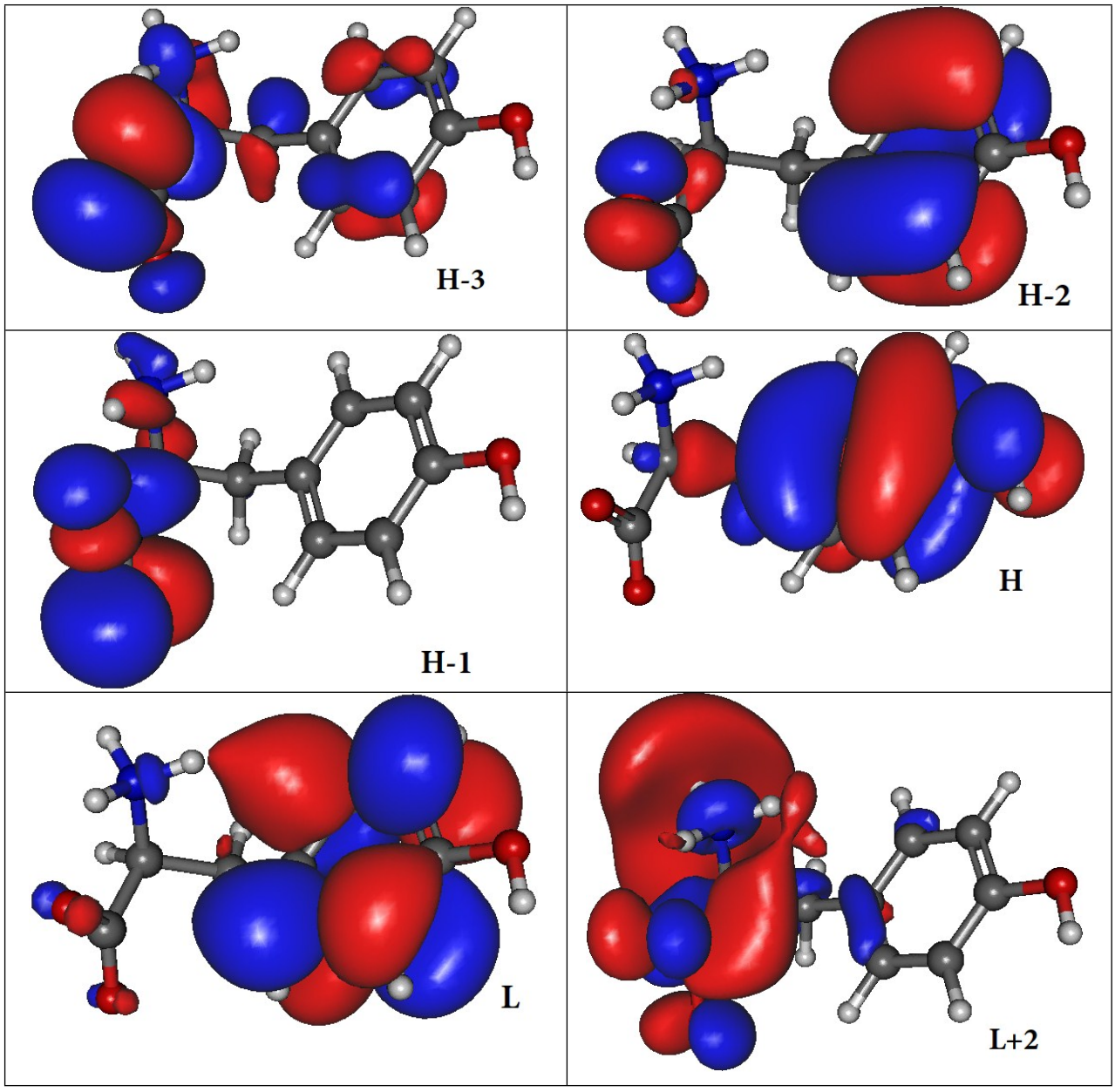


Fig. S1: Comparison between the electric dipole contribution to the Raman signal (left) and the chiral one (left) at the N K-edge with X polarized detection and a scattering angle of Pi/2.


H-3
H-2
H-1
H
L
L+2

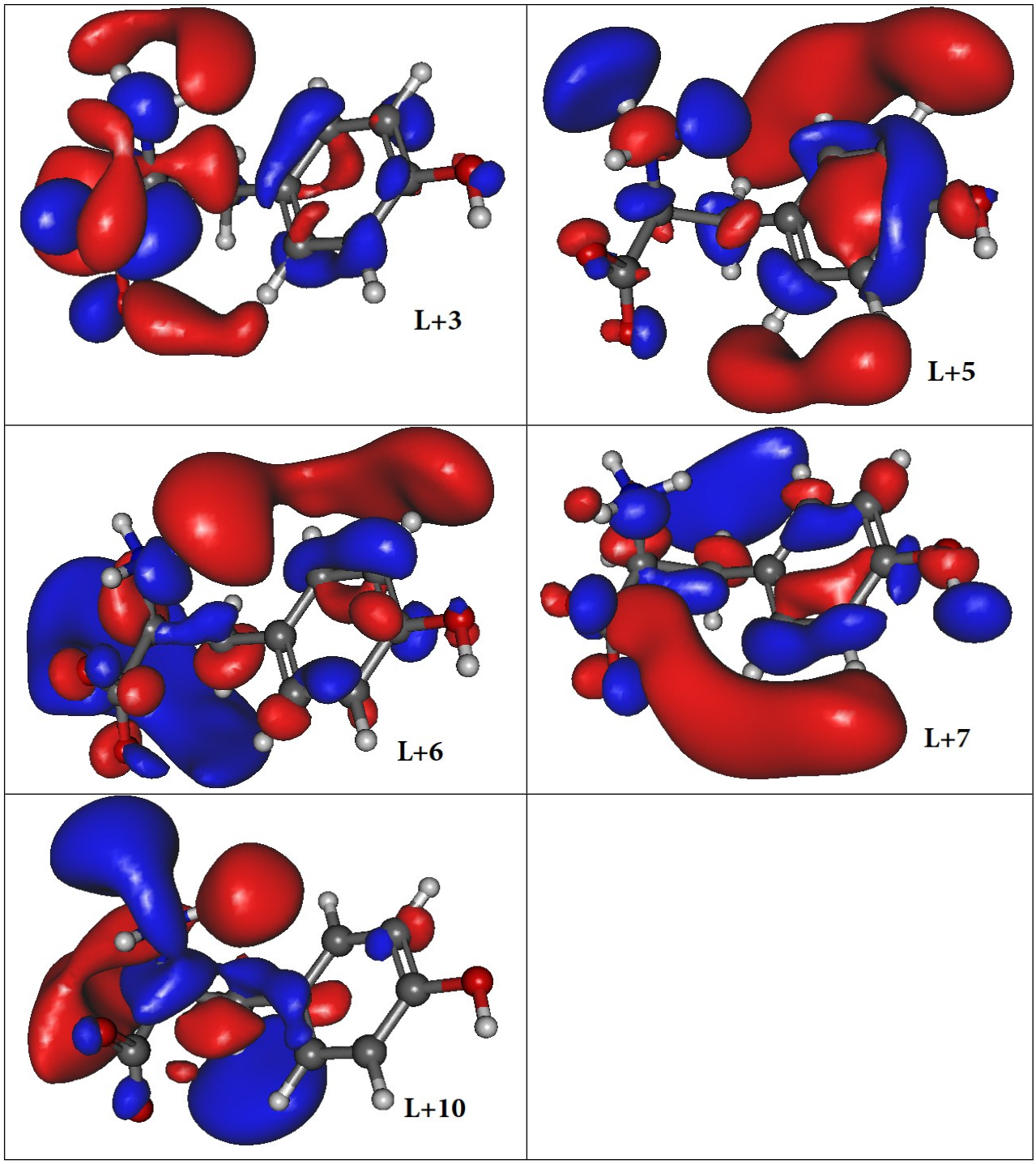


Figure S2. Important molecular orbitals of L-tyrosine at the B3LYP/cc-pVTZ level of theory using NWChem. The "H" label means HOMO and "L" means "LUMO". The surface is created using Avogadro [1] with the isovalue set to 0.02.

Excitation Type	Excitation Energy (eV)	From Transition Orbital	To Transition Orbital	CI-type Coefficient	Remark
Valence	6.0098	H-3	L	-0.90319	Strong absorption
Valence	6.2205	H-1	L+2	0.59471	Weak absorption
		H	L+2	0.58761	
Valence	6.6109	H-3	L+2	0.68940	Weak absorption
Valence	7.2136	H	L+5	0.43407	Weak absorption
		H-2	L	0.43115	
		H-2	L+2	0.39884	
		H	L+6	0.32173	
Valence	8.2969	H-2	L+6	0.72298	Weak absorption
Valence	8.3993	H-1	L+7	-0.76972	Weak absorption
N 1s	390.6113	N 1s	L	-0.99324	Weak absorption
N 1s	393.3490	N 1s	L+10	0.67898	Strong absorption
		N 1s	L+7	-0.42209	
O 1s	517.7787	O2,3 1s	L	-0.72925	Strong absorption
O 1s	518.2162	O2,3 1s	L	0.68284	Strong absorption
		O2,3 1s	L+2	0.55789	
O 1s	519.4231	O2,3 1s	L+3	-0.75292	Weak absorption
		O2,3 1s	L+2	-0.60031	
O 1s	519.4781	O2,3 1s	L+3	0.76487	Weak absorption
		O2,3 1s	L+2	0.57701	
O 1s	521.5083	O1 1s	L+2	0.99221	Strong absorption

Table S1. Representative valence and core excitations relevant to strong 2D ROA signals.

Reference

[1] Marcus D Hanwell, Donald E Curtis, David C Lonie, Tim Vandermeersch, Eva Zurek and Geoffrey R Hutchison; “Avogadro: An advanced semantic chemical editor, visualization, and analysis platform” Journal of Cheminformatics 2012, 4:17.