Supporting Information for

Ab initio static and molecular dynamics study of the absorption spectra of the 4-styrylpyridine photoswitch in its _cis_ and _trans_ forms

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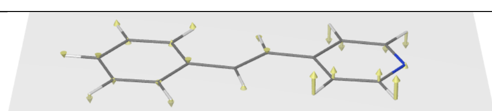
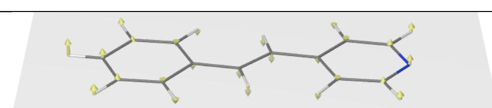
1 Vibrational normal coordinates and frequencies determined in the harmonic approximation for 4-styrylpyridine in the S_0 ground state, and Huang-Rhys factors calculated within the displaced harmonic oscillator approximation for the structural variations induced by the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ changes of states

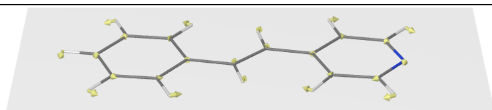
1.1 *Trans*-4-styrlpyridine: vibrational analysis in the ground state and $S_0 \rightarrow S_1$ Huang-Rhys factors (B3LYP/$\mathcal{G}$ results)

Table S1: Vibrational normal coordinates and frequencies obtained within the harmonic approximation for *trans*-4-styrylpyridine in the S_0 ground state. The $|Q_1|$'s are the magnitudes of the projections on the ground-state mass-weighted normal coordinates of the structural variation induced by the $S_0 \rightarrow S_1$ change of states, the $\mathcal{S}_1$'s are the associated Huang-Rhys factors (B3LYP/$\mathcal{G}$ results).

	
$\nu_1(a'') = 11$ cm^{-1}	$\nu_2(a'') = 56$ cm^{-1}
$\|Q_1\| = 0$ amu$^{1/2}$ Å	$\|Q_1\| = 0$ amu$^{1/2}$ Å
$\mathcal{S}_1 = 0$	$\mathcal{S}_1 = 0$

To be continued ...

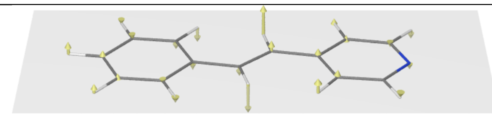
Table S1: *continued.*



$\nu_3(a') = 78\ \mathrm{cm}^{-1}$

$|Q_1| = 0.257\ \mathrm{amu}^{1/2}$ Å

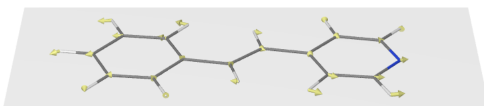
$\mathcal{S}_1 = 0.077$



$\nu_4(a'') = 88\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}$ Å

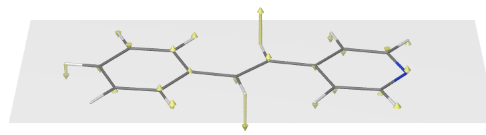
$\mathcal{S}_1 = 0$



$\nu_5(a') = 202\ \mathrm{cm}^{-1}$

$|Q_1| = 0.534\ \mathrm{amu}^{1/2}$ Å

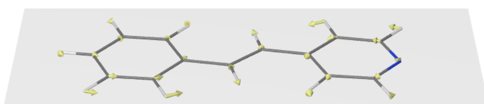
$\mathcal{S}_1 = 0.853$



$\nu_6(a'') = 226\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}$ Å

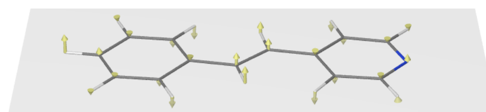
$\mathcal{S}_1 = 0$



$\nu_7(a') = 284\ \mathrm{cm}^{-1}$

$|Q_1| = 0.114\ \mathrm{amu}^{1/2}$ Å

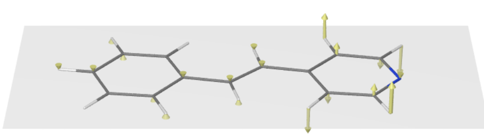
$\mathcal{S}_1 = 0.055$



$\nu_8(a'') = 286\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}$ Å

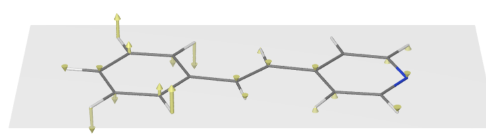
$\mathcal{S}_1 = 0$



$\nu_9(a'') = 390\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}$ Å

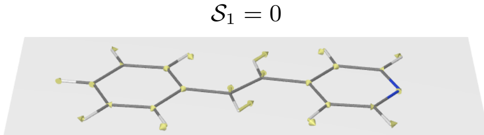
$\mathcal{S}_1 = 0$



$\nu_{10}(a'') = 409\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}$ Å

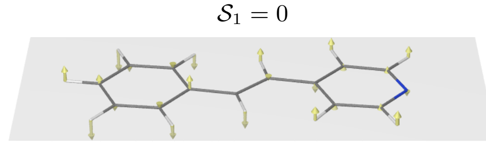
$\mathcal{S}_1 = 0$



$\nu_{11}(a') = 469\ \mathrm{cm}^{-1}$

$|Q_1| = 0.035\ \mathrm{amu}^{1/2}$ Å

$\mathcal{S}_1 = 0.008$



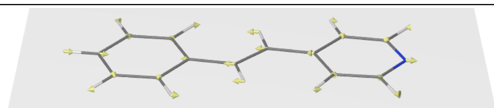
$\nu_{12}(a'') = 485\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}$ Å

$\mathcal{S}_1 = 0$

To be continued ...

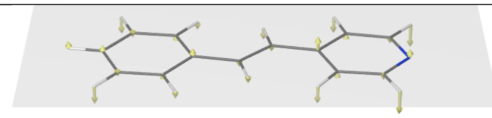
Table S1: *continued.*



$\nu_{13}(a') = 542\ \mathrm{cm}^{-1}$

$|Q_1| = 0.016\ \mathrm{amu}^{1/2}\ \text{Å}$

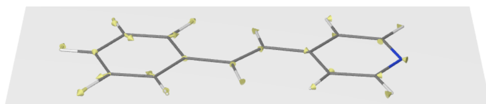
$\mathcal{S}_1 = 0.002$



$\nu_{14}(a'') = 558\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}\ \text{Å}$

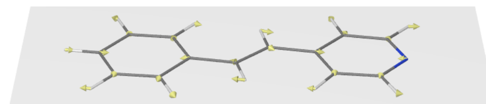
$\mathcal{S}_1 = 0$



$\nu_{15}(a') = 623\ \mathrm{cm}^{-1}$

$|Q_1| = 0.014\ \mathrm{amu}^{1/2}\ \text{Å}$

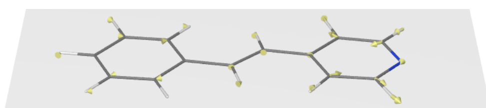
$\mathcal{S}_1 = 0.002$



$\nu_{16}(a') = 646\ \mathrm{cm}^{-1}$

$|Q_1| = 0.042\ \mathrm{amu}^{1/2}\ \text{Å}$

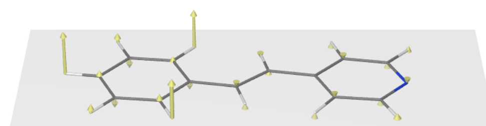
$\mathcal{S}_1 = 0.017$



$\nu_{17}(a') = 674\ \mathrm{cm}^{-1}$

$|Q_1| = 0.010\ \mathrm{amu}^{1/2}\ \text{Å}$

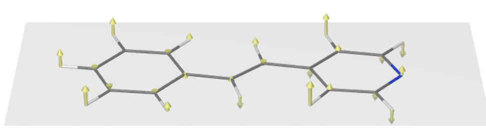
$\mathcal{S}_1 = 0.001$



$\nu_{18}(a) = 702\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}\ \text{Å}$

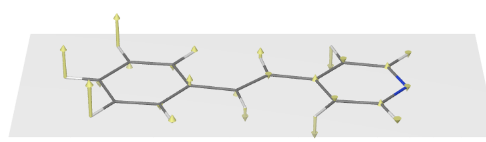
$\mathcal{S}_1 = 0$



$\nu_{19}(a'') = 749\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0$



$\nu_{20}(a'') = 774\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}\ \text{Å}$

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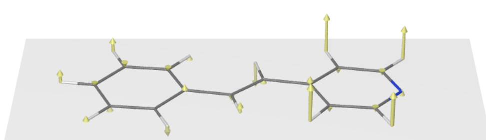
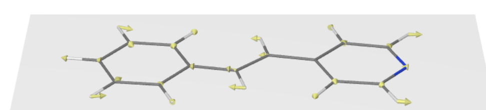


$\nu_{21}(a'') = 828\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0$



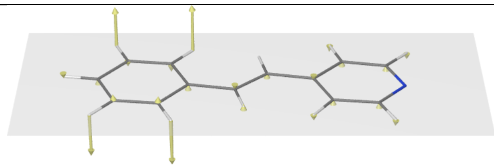
$\nu_{22}(a') = 838\ \mathrm{cm}^{-1}$

$|Q_1| = 0.025\ \mathrm{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0.008$

To be continued ...

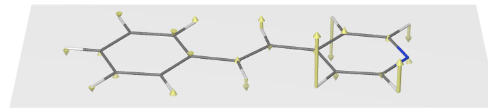
Table S1: *continued.*



$\nu_{23}(a'') = 853$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

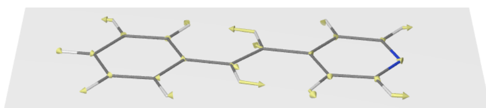
$\mathcal{S}_1 = 0$



$\nu_{24}(a) = 877$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

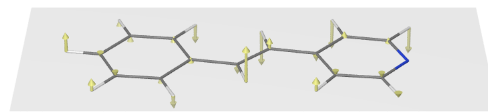
$\mathcal{S}_1 = 0$



$\nu_{25}(a') = 883$ cm^{-1}

$|Q_1| = 0.063$ amu$^{1/2}$ Å

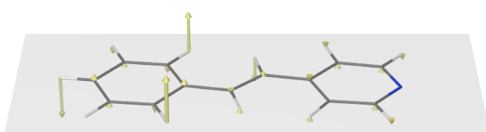
$\mathcal{S}_1 = 0.052$



$\nu_{26}(a'') = 897$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

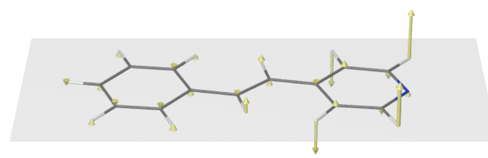
$\mathcal{S}_1 = 0$



$\nu_{27}(a'') = 934$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

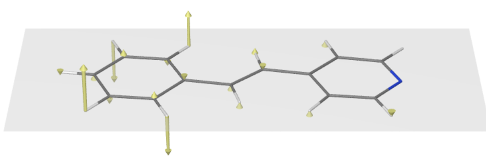
$\mathcal{S}_1 = 0$



$\nu_{28}(a'') = 971$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

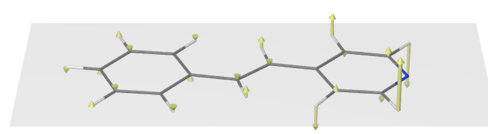
$\mathcal{S}_1 = 0$



$\nu_{29}(a'') = 988$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

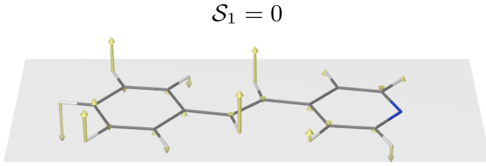
$\mathcal{S}_1 = 0$



$\nu_{30}(a'') =$ cm^{-1}

$|Q_1| = 995$ amu$^{1/2}$ Å

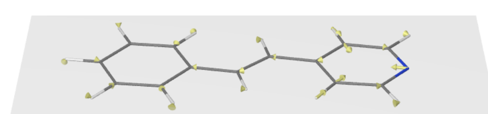
$\mathcal{S}_1 = 0$



$\nu_{31}(a'') = 999$ cm^{-1}

$|Q_1| = 0$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0$



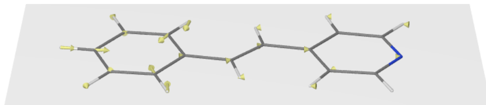
$\nu_{32}(a') = 1001$ cm^{-1}

$|Q_1| = 0.061$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.055$

To be continued ...

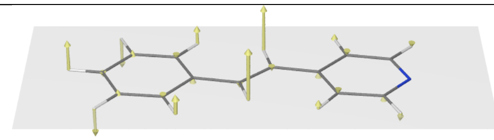
Table S1: *continued.*



$\nu_{33}(a') = 1005\ \mathrm{cm}^{-1}$

$|Q_1| = 0.061\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

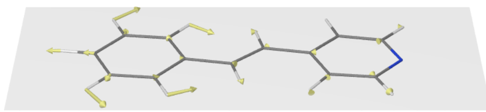
$\mathcal{S}_1 = 0.056$



$\nu_{34}(a'') = 1008\ \mathrm{cm}^{-1}$

$|Q_1| = 0\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

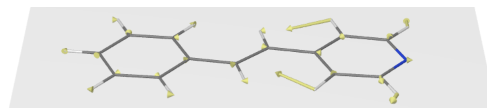
$\mathcal{S}_1 = 0$



$\nu_{35}(a') = 1046\ \mathrm{cm}^{-1}$

$|Q_1| = 0.005\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

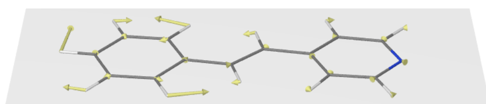
$\mathcal{S}_1 = 0.000$



$\nu_{36}(a') = 1088\ \mathrm{cm}^{-1}$

$|Q_1| = 0.018\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

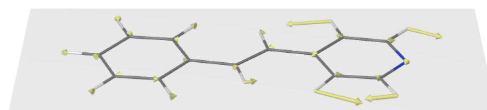
$\mathcal{S}_1 = 0.005$



$\nu_{37}(a') = 1101\ \mathrm{cm}^{-1}$

$|Q_1| = 0.008\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

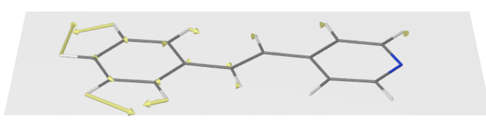
$\mathcal{S}_1 = 0.001$



$\nu_{38}(a') = 1117\ \mathrm{cm}^{-1}$

$|Q_1| = 0.017\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

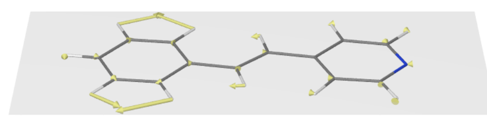
$\mathcal{S}_1 = 0.005$



$\nu_{39}(a') = 1181\ \mathrm{cm}^{-1}$

$|Q_1| = 0.020\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

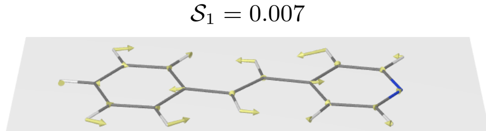
$\mathcal{S}_1 = 0.007$



$\nu_{40}(a') = 1200\ \mathrm{cm}^{-1}$

$|Q_1| = 0.048\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

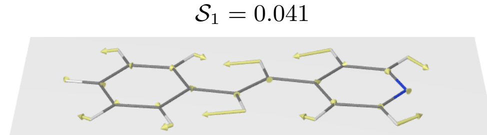
$\mathcal{S}_1 = 0.041$



$\nu_{41}(a') = 1215\ \mathrm{cm}^{-1}$

$|Q_1| = 0.059\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

$\mathcal{S}_1 = 0.063$



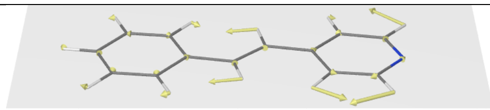
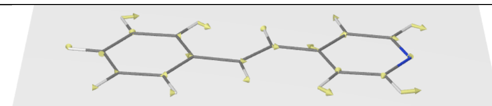
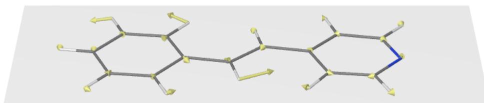
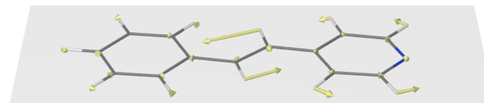
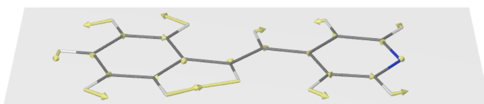
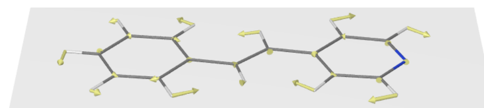
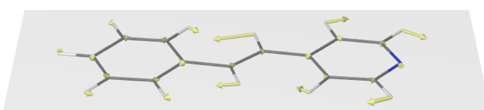
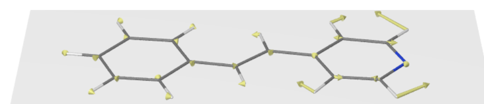
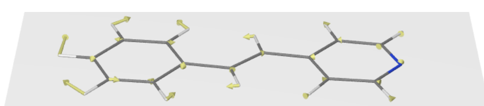
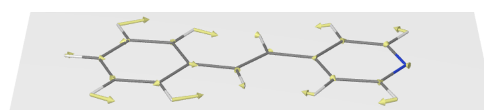
$\nu_{42}(a') = 1237\ \mathrm{cm}^{-1}$

$|Q_1| = 0.024\ \mathrm{amu}^{1/2}\ \mathrm{\AA}$

$\mathcal{S}_1 = 0.011$

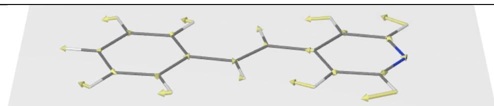
To be continued . . .

Table S1: *continued.*

	
$\nu_{43}(a') = 1252\ \mathrm{cm}^{-1}$	$\nu_{44}(a') = 1294\ \mathrm{cm}^{-1}$
$\lvert Q_1 \rvert = 0.018\ \mathrm{amu}^{1/2}\ \text{Å}$	$\lvert Q_1 \rvert = 0.001\ \mathrm{amu}^{1/2}\ \text{Å}$
$\mathcal{S}_1 = 0.006$	$\mathcal{S}_1 = 0.000$
	
$\nu_{45}(a') = 1321\ \mathrm{cm}^{-1}$	$\nu_{46}(a') = 1337\ \mathrm{cm}^{-1}$
$\lvert Q_1 \rvert = 0.026\ \mathrm{amu}^{1/2}\ \text{Å}$	$\lvert Q_1 \rvert = 0.047\ \mathrm{amu}^{1/2}\ \text{Å}$
$\mathcal{S}_1 = 0.013$	$\mathcal{S}_1 = 0.043$
	
$\nu_{47}(a') = 1357\ \mathrm{cm}^{-1}$	$\nu_{48}(a) = 1363\ \mathrm{cm}^{-1}$
$\lvert Q_1 \rvert = 0.065\ \mathrm{amu}^{1/2}\ \text{Å}$	$\lvert Q_1 \rvert = 0.020\ \mathrm{amu}^{1/2}\ \text{Å}$
$\mathcal{S}_1 = 0.085$	$\mathcal{S}_1 = 0.008$
	
$\nu_{49}(a') = 1375\ \mathrm{cm}^{-1}$	$\nu_{50}(a') = 1448\ \mathrm{cm}^{-1}$
$\lvert Q_1 \rvert = 0.034\ \mathrm{amu}^{1/2}\ \text{Å}$	$\lvert Q_1 \rvert = 0.027\ \mathrm{amu}^{1/2}\ \text{Å}$
$\mathcal{S}_1 = 0.023$	$\mathcal{S}_1 = 0.015$
	
$\nu_{51}(a') = 1474\ \mathrm{cm}^{-1}$	$\nu_{52}(a') = 1517\ \mathrm{cm}^{-1}$
$\lvert Q_1 \rvert = 0.031\ \mathrm{amu}^{1/2}\ \text{Å}$	$\lvert Q_1 \rvert = 0.033\ \mathrm{amu}^{1/2}\ \text{Å}$
$\mathcal{S}_1 = 0.021$	$\mathcal{S}_1 = 0.025$

To be continued ...

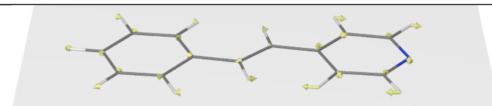
Table S1: *continued.*



$\nu_{53}(a') = 1529$ cm^{-1}

$|Q_1| = 0.005$ amu$^{1/2}$ Å

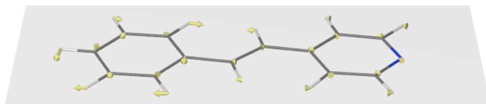
$\mathcal{S}_1 = 0.001$



$\nu_{54}(a') = 1597$ cm^{-1}

$|Q_1| = 0.060$ amu$^{1/2}$ Å

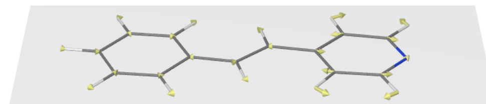
$\mathcal{S}_1 = 0.084$



$\nu_{55}(a') = 1619$ cm^{-1}

$|Q_1| = 0.039$ amu$^{1/2}$ Å

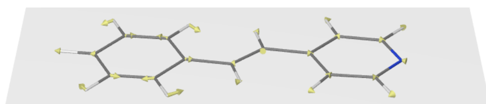
$\mathcal{S}_1 = 0.036$



$\nu_{56}(a') = 1636$ cm^{-1}

$|Q_1| = 0.087$ amu$^{1/2}$ Å

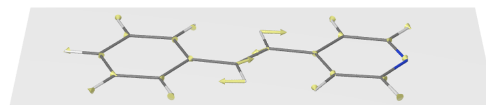
$\mathcal{S}_1 = 0.184$



$\nu_{57}(a') = 1649$ cm^{-1}

$|Q_1| = 0.055$ amu$^{1/2}$ Å

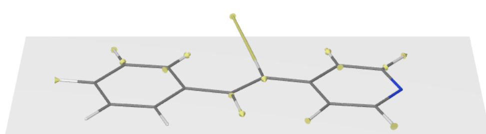
$\mathcal{S}_1 = 0.073$



$\nu_{58}(a') = 1690$ cm^{-1}

$|Q_1| = 0.124$ amu$^{1/2}$ Å

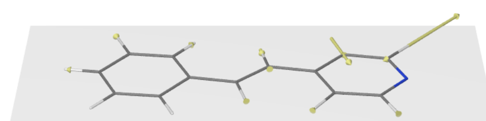
$\mathcal{S}_1 = 0.384$



$\nu_{59}(a') = 3158$ cm^{-1}

$|Q_1| = 0.004$ amu$^{1/2}$ Å

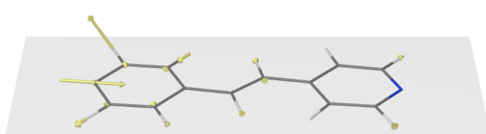
$\mathcal{S}_1 = 0.001$



$\nu_{60}(a') = 3166$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å

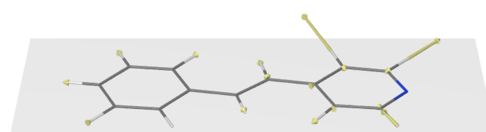
$\mathcal{S}_1 = 0.000$



$\nu_{61}(a') = 3174$ cm^{-1}

$|Q_1| = 0.000$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$



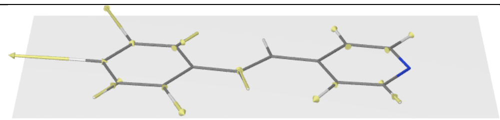
$\nu_{62}(a') = 3185$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$

To be continued ...

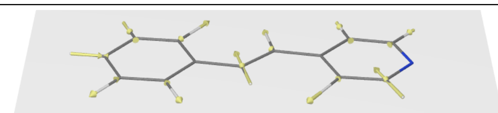
Table S1: *continued.*



$\nu_{63}(a') = 3188$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å

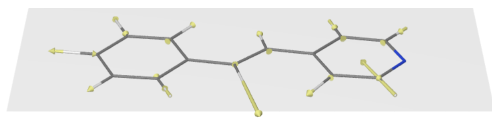
$\mathcal{S}_1 = 0.000$



$\nu_{64}(a') = 3189$ cm^{-1}

$|Q_1| = 0.002$ amu$^{1/2}$ Å

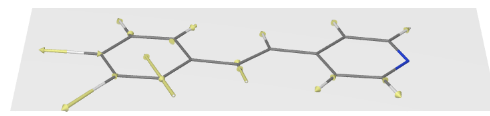
$\mathcal{S}_1 = 0.000$



$\nu_{65}(a') = 3191$ cm^{-1}

$|Q_1| = 0.002$ amu$^{1/2}$ Å

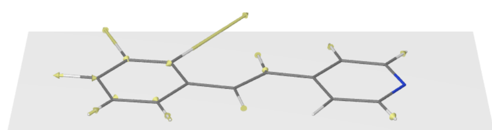
$\mathcal{S}_1 = 0.000$



$\nu_{66}(a') = 3198$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å

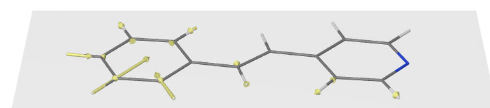
$\mathcal{S}_1 = 0.000$



$\nu_{67}(a') = 3205$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å

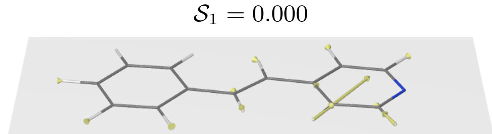
$\mathcal{S}_1 = 0.000$



$\nu_{68}(a') = 3216$ cm^{-1}

$|Q_1| = 0.002$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$



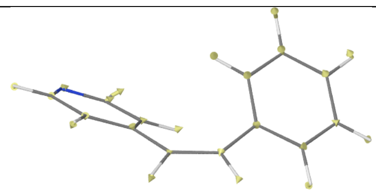
$\nu_{69}(a') = 3225$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$

1.2 *Cis*-4-styrlpyridine: vibrational analysis in the ground state and $S_0 \to S_1, S_2$ Huang-Rhys factors (BOP/$\mathcal{G}$ results)

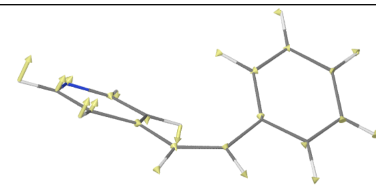
Table S2: Vibrational normal coordinates and frequencies obtained within the harmonic approximation for *cis*-4-styrylpyridine in the S_0 ground state. The $|Q_I|$'s are the magnitudes of the projections on the ground-state mass-weighted normal coordinates of the structural variation induced by the $S_0 \to S_I$ change of states, the $\mathcal{S}_I$'s are the associated Huang-Rhys factors ($I = 1, 2$; BOP/$\mathcal{G}$ results).



$\nu_1(a) = 40\ \mathrm{cm}^{-1}$

$|Q_1| = 0.286$ amu$^{1/2}$ Å $|Q_2| = 1.457$ amu$^{1/2}$ Å

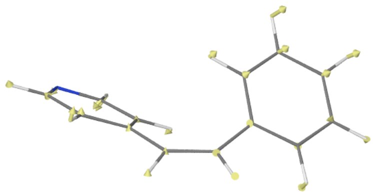
$\mathcal{S}_1 = 0.048$ $\mathcal{S}_2 = 1.253$



$\nu_2(a) = 48\ \mathrm{cm}^{-1}$

$|Q_1| = 0.961$ amu$^{1/2}$ Å $|Q_2| = 1.860$ amu$^{1/2}$ Å

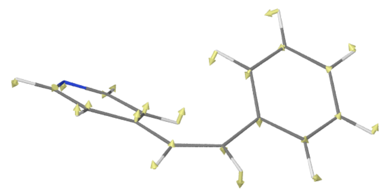
$\mathcal{S}_1 = 0.665$ $\mathcal{S}_2 = 2.488$



$\nu_3(a) = 80\ \mathrm{cm}^{-1}$

$|Q_1| = 0.239$ amu$^{1/2}$ Å $|Q_2| = 1.800$ amu$^{1/2}$ Å

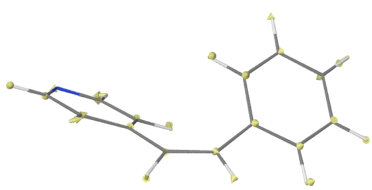
$\mathcal{S}_1 = 0.068$ $\mathcal{S}_2 = 3.865$



$\nu_4(a) = 155\ \mathrm{cm}^{-1}$

$|Q_1| = 0.721$ amu$^{1/2}$ Å $|Q_2| = 1.062$ amu$^{1/2}$ Å

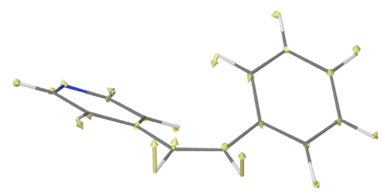
$\mathcal{S}_1 = 1.198$ $\mathcal{S}_2 = 2.597$



$\nu_5(a) = 156\ \mathrm{cm}^{-1}$

$|Q_1| = 0.404$ amu$^{1/2}$ Å $|Q_2| = 0.803$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.378$ $\mathcal{S}_2 = 1.495$



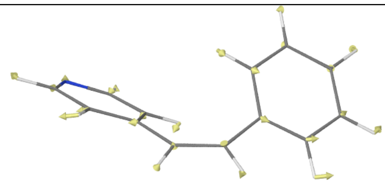
$\nu_6(a) = 237\ \mathrm{cm}^{-1}$

$|Q_1| = 0.116$ amu$^{1/2}$ Å $|Q_2| = 0.001$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.048$ $\mathcal{S}_2 = 0.000$

To be continued ...

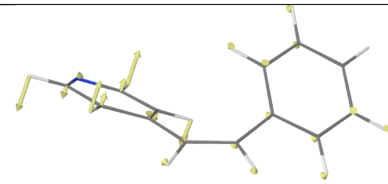
Table S2: *continued.*



$\nu_7(a) = 259$ cm^{-1}

$|Q_1| = 0.147$ amu$^{1/2}$ Å $|Q_2| = 0.169$ amu$^{1/2}$ Å

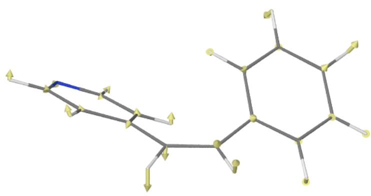
$\mathcal{S}_1 = 0.083$ $\mathcal{S}_2 = 0.109$



$\nu_8(a) = 372$ cm^{-1}

$|Q_1| = 0.027$ amu$^{1/2}$ Å $|Q_2| = 0.068$ amu$^{1/2}$ Å

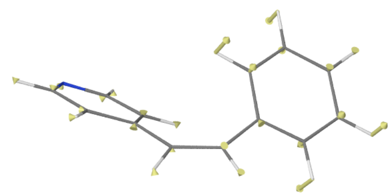
$\mathcal{S}_1 = 0.004$ $\mathcal{S}_2 = 0.025$



$\nu_9(a) = 389$ cm^{-1}

$|Q_1| = 0.398$ amu$^{1/2}$ Å $|Q_2| = 0.599$ amu$^{1/2}$ Å

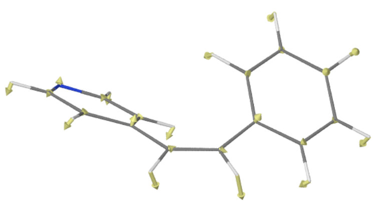
$\mathcal{S}_1 = 0.914$ $\mathcal{S}_2 = 2.074$



$\nu_{10}(a) = 399$ cm^{-1}

$|Q_1| = 0.072$ amu$^{1/2}$ Å $|Q_2| = 0.089$ amu$^{1/2}$ Å

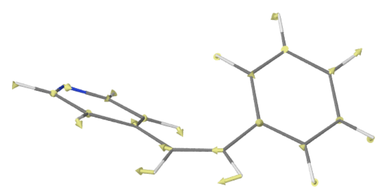
$\mathcal{S}_1 = 0.030$ $\mathcal{S}_2 = 0.046$



$\nu_{11}(a) = 451$ cm^{-1}

$|Q_1| = 0.009$ amu$^{1/2}$ Å $|Q_2| = 0.101$ amu$^{1/2}$ Å

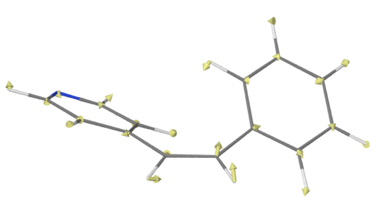
$\mathcal{S}_1 = 0.001$ $\mathcal{S}_2 = 0.069$



$\nu_{12}(a) = 495$ cm^{-1}

$|Q_1| = 0.260$ amu$^{1/2}$ Å $|Q_2| = 0.124$ amu$^{1/2}$ Å

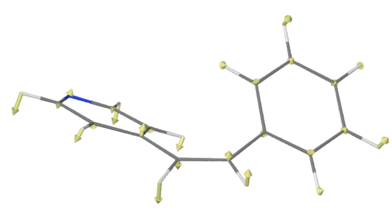
$\mathcal{S}_1 = 0.494$ $\mathcal{S}_2 = 0.114$



$\nu_{13}(a) = 508$ cm^{-1}

$|Q_1| = 0.040$ amu$^{1/2}$ Å $|Q_2| = 0.016$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.012$ $\mathcal{S}_2 = 0.002$



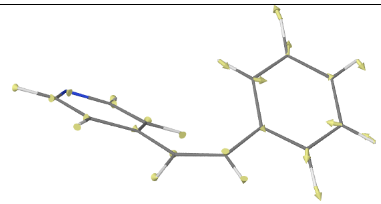
$\nu_{14}(a) = 564$ cm^{-1}

$|Q_1| = 0.218$ amu$^{1/2}$ Å $|Q_2| = 0.280$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.396$ $\mathcal{S}_2 = 0.657$

To be continued ...

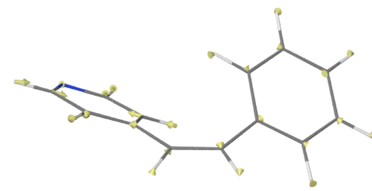
Table S2: *continued.*



$\nu_{15}(a) = 608$ cm^{-1}

$|Q_1| = 0.025$ amu$^{1/2}$ Å $|Q_2| = 0.023$ amu$^{1/2}$ Å

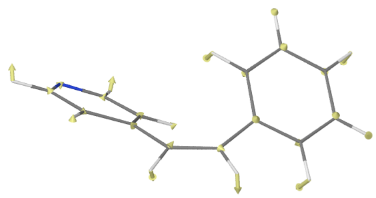
$\mathcal{S}_1 = 0.006$ $\mathcal{S}_2 = 0.005$



$\nu_{16}(a) = 654$ cm^{-1}

$|Q_1| = 0.064$ amu$^{1/2}$ Å $|Q_2| = 0.007$ amu$^{1/2}$ Å

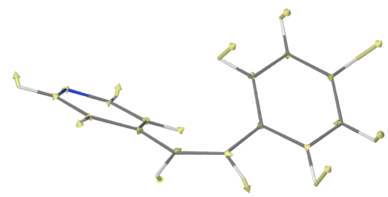
$\mathcal{S}_1 = 0.040$ $\mathcal{S}_2 = 0.001$



$\nu_{17}(a) = 680$ cm^{-1}

$|Q_1| = 0.074$ amu$^{1/2}$ Å $|Q_2| = 0.024$ amu$^{1/2}$ Å

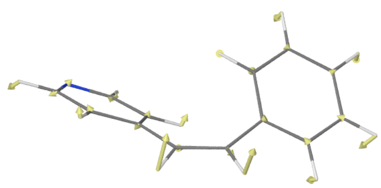
$\mathcal{S}_1 = 0.055$ $\mathcal{S}_2 = 0.006$



$\nu_{18}(a) = 691$ cm^{-1}

$|Q_1| = 0.067$ amu$^{1/2}$ Å $|Q_2| = 0.003$ amu$^{1/2}$ Å

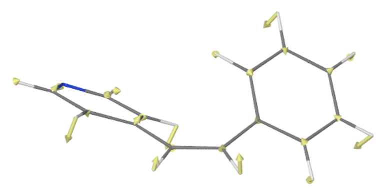
$\mathcal{S}_1 = 0.047$ $\mathcal{S}_2 = 0.000$



$\nu_{19}(a) = 722$ cm^{-1}

$|Q_1| = 0.073$ amu$^{1/2}$ Å $|Q_2| = 0.074$ amu$^{1/2}$ Å

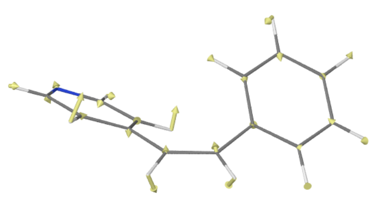
$\mathcal{S}_1 = 0.057$ $\mathcal{S}_2 = 0.059$



$\nu_{20}(a) = 734$ cm^{-1}

$|Q_1| = 0.187$ amu$^{1/2}$ Å $|Q_2| = 0.112$ amu$^{1/2}$ Å

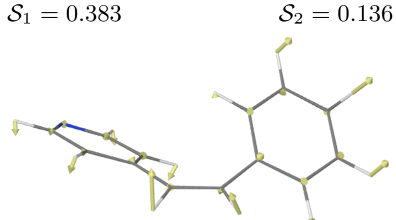
$\mathcal{S}_1 = 0.383$ $\mathcal{S}_2 = 0.136$



$\nu_{21}(a) = 747$ cm^{-1}

$|Q_1| = 0.103$ amu$^{1/2}$ Å $|Q_2| = 0.005$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.118$ $\mathcal{S}_2 = 0.000$



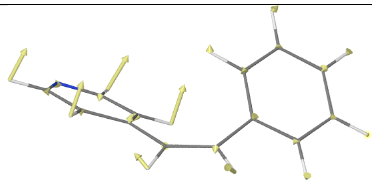
$\nu_{22}(a) = 772$ cm^{-1}

$|Q_1| = 0.062$ amu$^{1/2}$ Å $|Q_2| = 0.081$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.045$ $\mathcal{S}_2 = 0.074$

To be continued ...

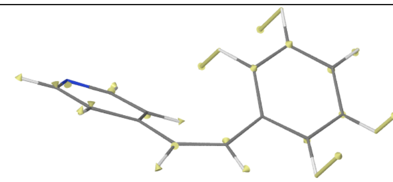
Table S2: *continued.*



$\nu_{23}(a) = 811$ cm^{-1}

$|Q_1| = 0.120$ amu$^{1/2}$ Å $|Q_2| = 0.085$ amu$^{1/2}$ Å

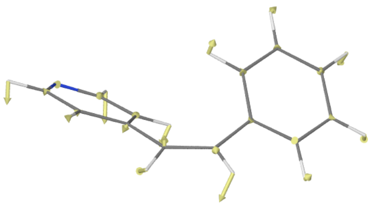
$\mathcal{S}_1 = 0.174$ $\mathcal{S}_2 = 0.087$



$\nu_{24}(a) = 834$ cm^{-1}

$|Q_1| = 0.041$ amu$^{1/2}$ Å $|Q_2| = 0.060$ amu$^{1/2}$ Å

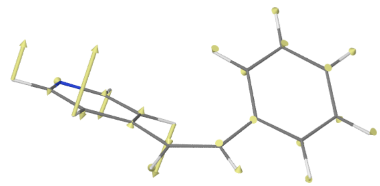
$\mathcal{S}_1 = 0.021$ $\mathcal{S}_2 = 0.045$



$\nu_{25}(a) = 860$ cm^{-1}

$|Q_1| = 0.072$ amu$^{1/2}$ Å $|Q_2| = 0.014$ amu$^{1/2}$ Å

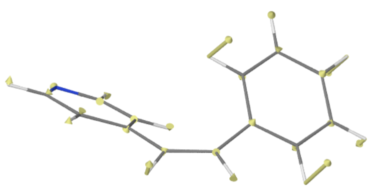
$\mathcal{S}_1 = 0.066$ $\mathcal{S}_2 = 0.002$



$\nu_{26}(a) = 864$ cm^{-1}

$|Q_1| = 0.026$ amu$^{1/2}$ Å $|Q_2| = 0.007$ amu$^{1/2}$ Å

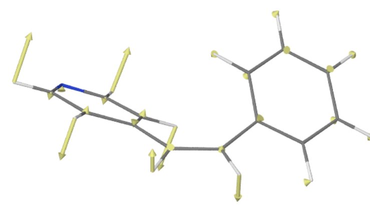
$\mathcal{S}_1 = 0.009$ $\mathcal{S}_2 = 0.001$



$\nu_{27}(a) = 908$ cm^{-1}

$|Q_1| = 0.063$ amu$^{1/2}$ Å $|Q_2| = 0.085$ amu$^{1/2}$ Å

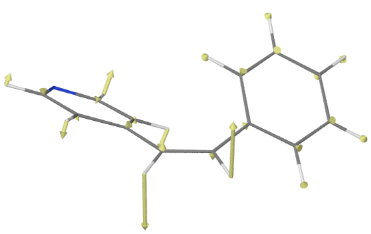
$\mathcal{S}_1 = 0.053$ $\mathcal{S}_2 = 0.096$



$\nu_{28}(a) = 938$ cm^{-1}

$|Q_1| = 0.031$ amu$^{1/2}$ Å $|Q_2| = 0.103$ amu$^{1/2}$ Å

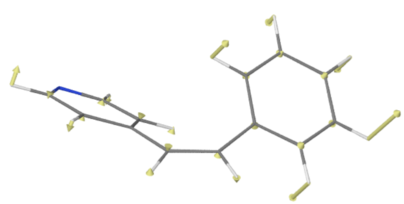
$\mathcal{S}_1 = 0.013$ $\mathcal{S}_2 = 0.149$



$\nu_{29}(a) = 946$ cm^{-1}

$|Q_1| = 0.102$ amu$^{1/2}$ Å $|Q_2| = 0.148$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.145$ $\mathcal{S}_2 = 0.306$



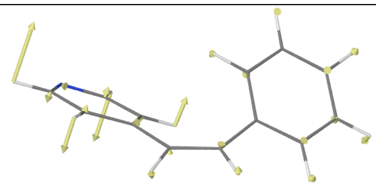
$\nu_{30}(a) = 951$ cm^{-1}

$|Q_1| = 0.031$ amu$^{1/2}$ Å $|Q_2| = 0.040$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.013$ $\mathcal{S}_2 = 0.023$

To be continued ...

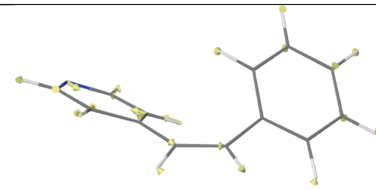
Table S2: *continued.*



$\nu_{31}(a) = 955$ cm^{-1}

$|Q_1| = 0.018$ amu$^{1/2}$ Å $|Q_2| = 0.082$ amu$^{1/2}$ Å

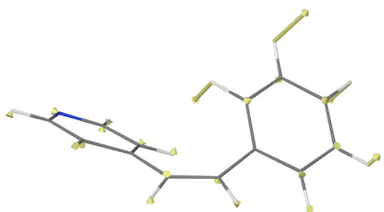
$\mathcal{S}_1 = 0.005$ $\mathcal{S}_2 = 0.096$



$\nu_{32}(a) = 962$ cm^{-1}

$|Q_1| = 0.281$ amu$^{1/2}$ Å $|Q_2| = 0.061$ amu$^{1/2}$ Å

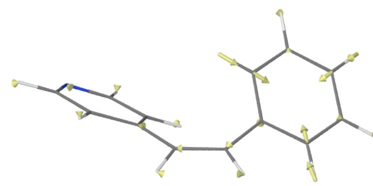
$\mathcal{S}_1 = 1.130$ $\mathcal{S}_2 = 0.053$



$\nu_{33}(a) = 971$ cm^{-1}

$|Q_1| = 0.000$ amu$^{1/2}$ Å $|Q_2| = 0.039$ amu$^{1/2}$ Å

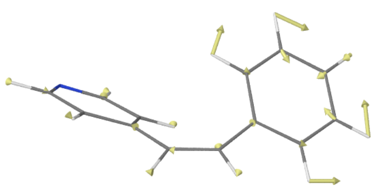
$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.022$



$\nu_{34}(a) = 975$ cm^{-1}

$|Q_1| = 0.045$ amu$^{1/2}$ Å $|Q_2| = 0.019$ amu$^{1/2}$ Å

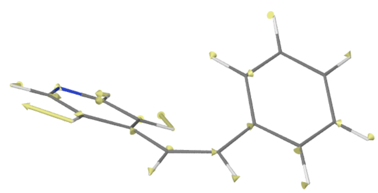
$\mathcal{S}_1 = 0.029$ $\mathcal{S}_2 = 0.005$



$\nu_{35}(a) = 1013$ cm^{-1}

$|Q_1| = 0.016$ amu$^{1/2}$ Å $|Q_2| = 0.032$ amu$^{1/2}$ Å

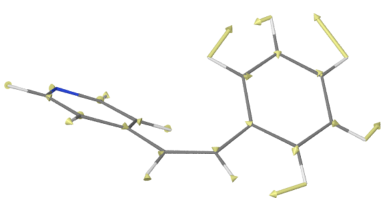
$\mathcal{S}_1 = 0.004$ $\mathcal{S}_2 = 0.015$



$\nu_{36}(a) = 1055$ cm^{-1}

$|Q_1| = 0.011$ amu$^{1/2}$ Å $|Q_2| = 0.029$ amu$^{1/2}$ Å

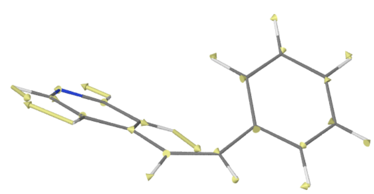
$\mathcal{S}_1 = 0.002$ $\mathcal{S}_2 = 0.013$



$\nu_{37}(a) = 1072$ cm^{-1}

$|Q_1| = 0.013$ amu$^{1/2}$ Å $|Q_2| = 0.003$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.003$ $\mathcal{S}_2 = 0.000$



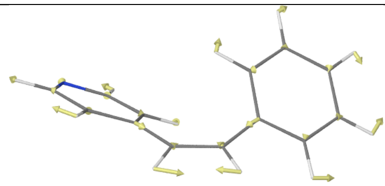
$\nu_{38}(a) = 1081$ cm^{-1}

$|Q_1| = 0.020$ amu$^{1/2}$ Å $|Q_2| = 0.016$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.006$ $\mathcal{S}_2 = 0.004$

To be continued ...

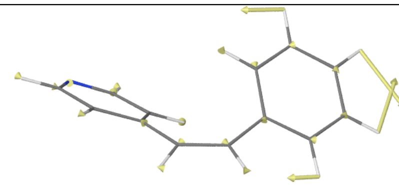
Table S2: *continued.*



$\nu_{39}(a) = 1139$ cm^{-1}

$|Q_1| = 0.130$ amu$^{1/2}$ Å $|Q_2| = 0.068$ amu$^{1/2}$ Å

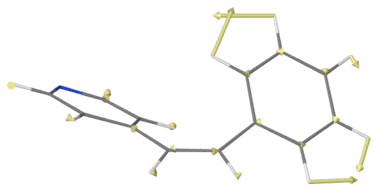
$\mathcal{S}_1 = 0.286$ $\mathcal{S}_2 = 0.077$



$\nu_{40}(a) = 1157$ cm^{-1}

$|Q_1| = 0.029$ amu$^{1/2}$ Å $|Q_2| = 0.037$ amu$^{1/2}$ Å

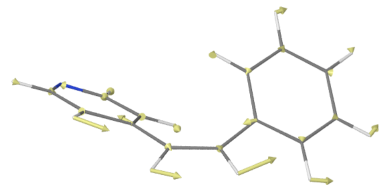
$\mathcal{S}_1 = 0.014$ $\mathcal{S}_2 = 0.023$



$\nu_{41}(a) = 1173$ cm^{-1}

$|Q_1| = 0.019$ amu$^{1/2}$ Å $|Q_2| = 0.026$ amu$^{1/2}$ Å

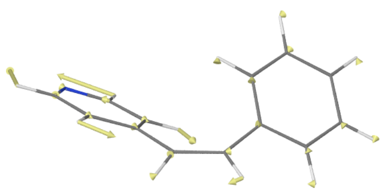
$\mathcal{S}_1 = 0.006$ $\mathcal{S}_2 = 0.011$



$\nu_{42}(a) = 1193$ cm^{-1}

$|Q_1| = 0.076$ amu$^{1/2}$ Å $|Q_2| = 0.019$ amu$^{1/2}$ Å

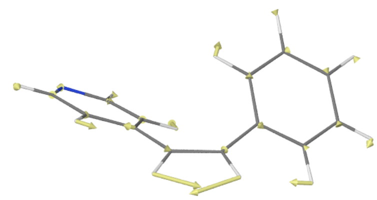
$\mathcal{S}_1 = 0.101$ $\mathcal{S}_2 = 0.006$



$\nu_{43}(a) = 1210$ cm^{-1}

$|Q_1| = 0.020$ amu$^{1/2}$ Å $|Q_2| = 0.021$ amu$^{1/2}$ Å

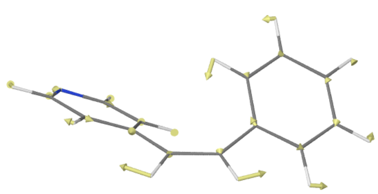
$\mathcal{S}_1 = 0.007$ $\mathcal{S}_2 = 0.008$



$\nu_{44}(a) = 1234$ cm^{-1}

$|Q_1| = 0.033$ amu$^{1/2}$ Å $|Q_2| = 0.008$ amu$^{1/2}$ Å

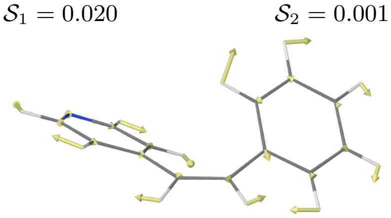
$\mathcal{S}_1 = 0.020$ $\mathcal{S}_2 = 0.001$



$\nu_{45}(a) = 1276$ cm^{-1}

$|Q_1| = 0.023$ amu$^{1/2}$ Å $|Q_2| = 0.002$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.010$ $\mathcal{S}_2 = 0.000$



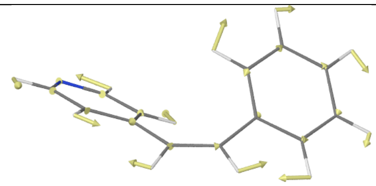
$\nu_{46}(a) = 1310$ cm^{-1}

$|Q_1| = 0.001$ amu$^{1/2}$ Å $|Q_2| = 0.001$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.000$

To be continued ...

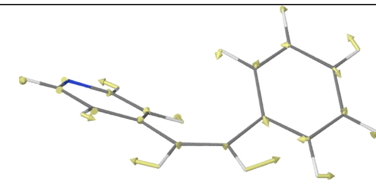
Table S2: *continued.*



$\nu_{47}(a) = 1327\ \mathrm{cm}^{-1}$

$|Q_1| = 0.039\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.037\ \mathrm{amu}^{1/2}$ Å

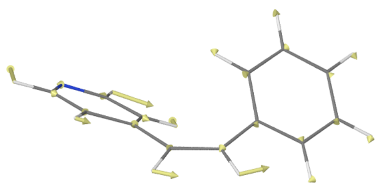
$\mathcal{S}_1 = 0.030$ $\mathcal{S}_2 = 0.027$



$\nu_{48}(a) = 1332\ \mathrm{cm}^{-1}$

$|Q_1| = 0.020\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.002\ \mathrm{amu}^{1/2}$ Å

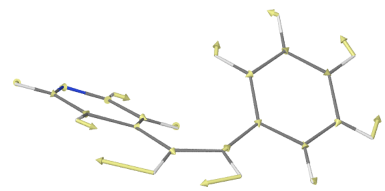
$\mathcal{S}_1 = 0.008$ $\mathcal{S}_2 = 0.000$



$\nu_{49}(a) = 1396\ \mathrm{cm}^{-1}$

$|Q_1| = 0.010\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.021\ \mathrm{amu}^{1/2}$ Å

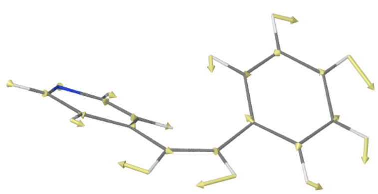
$\mathcal{S}_1 = 0.002$ $\mathcal{S}_2 = 0.009$



$\nu_{50}(a) = 1410\ \mathrm{cm}^{-1}$

$|Q_1| = 0.010\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.021\ \mathrm{amu}^{1/2}$ Å

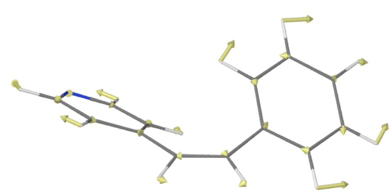
$\mathcal{S}_1 = 0.002$ $\mathcal{S}_2 = 0.009$



$\nu_{51}(a) = 1431\ \mathrm{cm}^{-1}$

$|Q_1| = 0.015\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.027\ \mathrm{amu}^{1/2}$ Å

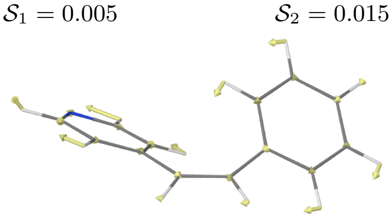
$\mathcal{S}_1 = 0.005$ $\mathcal{S}_2 = 0.015$



$\nu_{52}(a) = 1467\ \mathrm{cm}^{-1}$

$|Q_1| = 0.023\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.044\ \mathrm{amu}^{1/2}$ Å

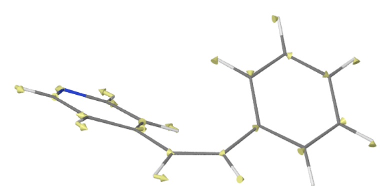
$\mathcal{S}_1 = 0.011$ $\mathcal{S}_2 = 0.042$



$\nu_{53}(a) = 1472\ \mathrm{cm}^{-1}$

$|Q_1| = 0.006\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.010\ \mathrm{amu}^{1/2}$ Å

$\mathcal{S}_1 = 0.001$ $\mathcal{S}_2 = 0.002$



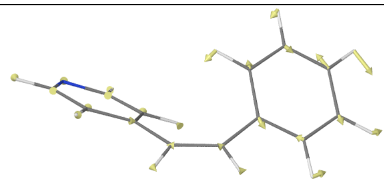
$\nu_{54}(a) = 1522\ \mathrm{cm}^{-1}$

$|Q_1| = 0.036\ \mathrm{amu}^{1/2}$ Å $|Q_2| = 0.056\ \mathrm{amu}^{1/2}$ Å

$\mathcal{S}_1 = 0.029$ $\mathcal{S}_2 = 0.070$

To be continued ...

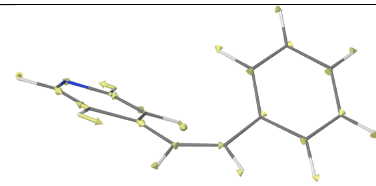
Table S2: *continued.*



$\nu_{55}(a) = 1555$ cm^{-1}

$|Q_1| = 0.020$ amu$^{1/2}$ Å $|Q_2| = 0.048$ amu$^{1/2}$ Å

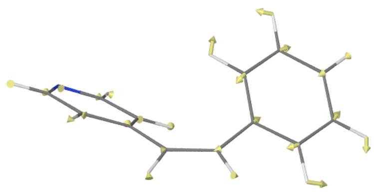
$\mathcal{S}_1 = 0.010$ $\mathcal{S}_2 = 0.052$



$\nu_{56}(a) = 1566$ cm^{-1}

$|Q_1| = 0.009$ amu$^{1/2}$ Å $|Q_2| = 0.054$ amu$^{1/2}$ Å

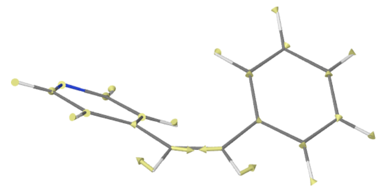
$\mathcal{S}_1 = 0.002$ $\mathcal{S}_2 = 0.069$



$\nu_{57}(a) = 1579$ cm^{-1}

$|Q_1| = 0.056$ amu$^{1/2}$ Å $|Q_2| = 0.046$ amu$^{1/2}$ Å

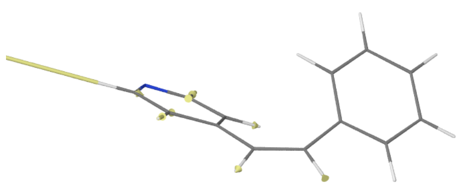
$\mathcal{S}_1 = 0.074$ $\mathcal{S}_2 = 0.049$



$\nu_{58}(a) = 1607$ cm^{-1}

$|Q_1| = 0.074$ amu$^{1/2}$ Å $|Q_2| = 0.053$ amu$^{1/2}$ Å

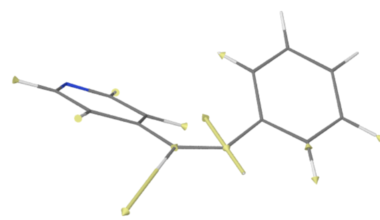
$\mathcal{S}_1 = 0.129$ $\mathcal{S}_2 = 0.066$



$\nu_{59}(a) = 3074$ cm^{-1}

$|Q_1| = 0.016$ amu$^{1/2}$ Å $|Q_2| = 0.005$ amu$^{1/2}$ Å

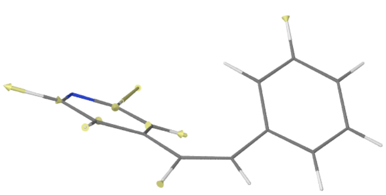
$\mathcal{S}_1 = 0.012$ $\mathcal{S}_2 = 0.001$



$\nu_{60}(a) = 3081$ cm^{-1}

$|Q_1| = 0.006$ amu$^{1/2}$ Å $|Q_2| = 0.006$ amu$^{1/2}$ Å

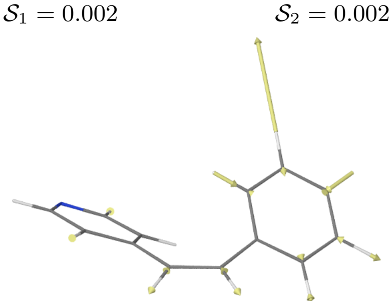
$\mathcal{S}_1 = 0.002$ $\mathcal{S}_2 = 0.002$



$\nu_{61}(a) = 3081$ cm^{-1}

$|Q_1| = 0.012$ amu$^{1/2}$ Å $|Q_2| = 0.008$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.007$ $\mathcal{S}_2 = 0.003$



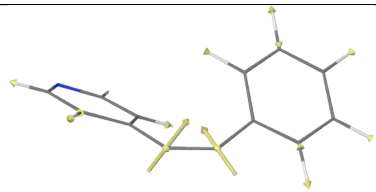
$\nu_{62}(a) = 3102$ cm^{-1}

$|Q_1| = 0.000$ amu$^{1/2}$ Å $|Q_2| = 0.000$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.000$

To be continued ...

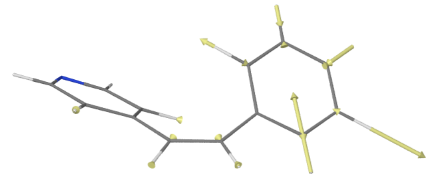
Table S2: *continued.*



$\nu_{63}(a) = 3102\ \text{cm}^{-1}$

$|Q_1| = 0.019\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.037\ \text{amu}^{1/2}\ \text{Å}$

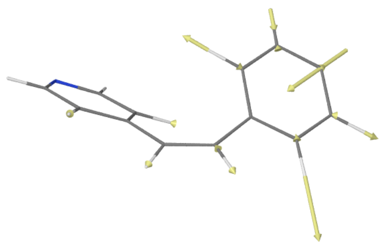
$\mathcal{S}_1 = 0.016$ $\mathcal{S}_2 = 0.065$



$\nu_{64}(a) = 3117\ \text{cm}^{-1}$

$|Q_1| = 0.002\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.006\ \text{amu}^{1/2}\ \text{Å}$

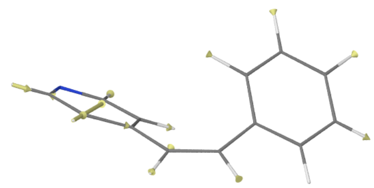
$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.001$



$\nu_{65}(a) = 3124\ \text{cm}^{-1}$

$|Q_1| = 0.000\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.002\ \text{amu}^{1/2}\ \text{Å}$

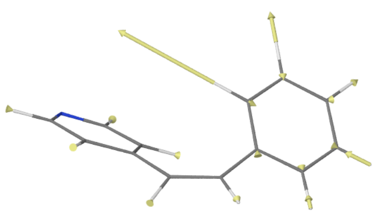
$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.000$



$\nu_{66}(a) = 3126\ \text{cm}^{-1}$

$|Q_1| = 0.011\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.012\ \text{amu}^{1/2}\ \text{Å}$

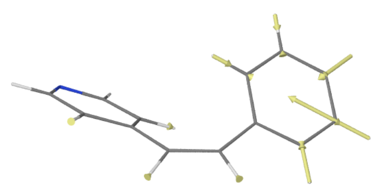
$\mathcal{S}_1 = 0.006$ $\mathcal{S}_2 = 0.006$



$\nu_{67}(a) = 3133\ \text{cm}^{-1}$

$|Q_1| = 0.000\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.010\ \text{amu}^{1/2}\ \text{Å}$

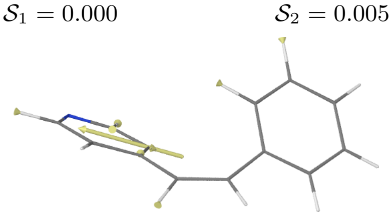
$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.005$



$\nu_{68}(a) = 3143\ \text{cm}^{-1}$

$|Q_1| = 0.000\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.014\ \text{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0.000$ $\mathcal{S}_2 = 0.009$



$\nu_{69}(a) = 3165\ \text{cm}^{-1}$

$|Q_1| = 0.015\ \text{amu}^{1/2}\ \text{Å}$ $|Q_2| = 0.018\ \text{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0.010$ $\mathcal{S}_2 = 0.015$

1.3 *Cis*-4-styrlpyridine: vibrational analysis in the ground state, optimised S_1 geometry and $\mathrm{S}_0 \rightarrow \mathrm{S}_1$ Huang-Rhys factors (B3LYP/$\mathcal{G}$ results)

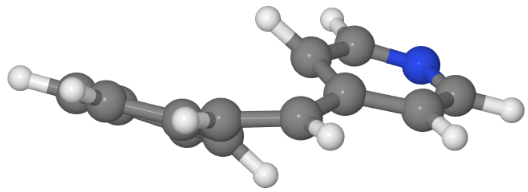
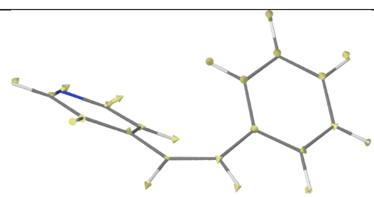
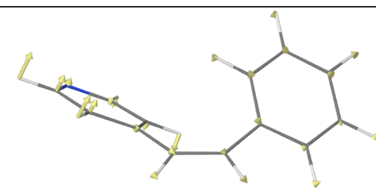
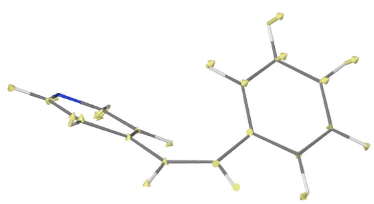
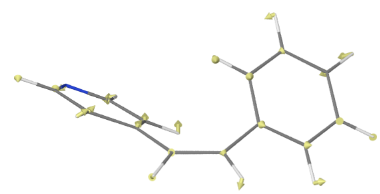


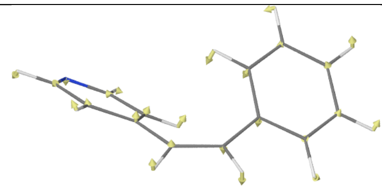
Figure S1: Optimised B3LYP/$\mathcal{G}$ geometry of cis-4-styrylpyridine in the S_1 state.

Table S3: Vibrational normal coordinates and frequencies obtained within the harmonic approximation for *cis*-4-styrylpyridine in the S_0 ground state. The $|Q_1|$'s are the magnitudes of the projections on the ground-state mass-weighted normal coordinates of the structural variation induced by the $\mathrm{S}_0 \rightarrow \mathrm{S}_1$ change of states, the $\mathcal{S}_1$'s are the associated Huang-Rhys factors (B3LYP/$\mathcal{G}$ results).

	
$\nu_1(a) = 37$ cm^{-1}	$\nu_2(a) = 51$ cm^{-1}
$\lvert Q_1 \rvert = 3.232$ amu$^{1/2}$ Å	$\lvert Q_1 \rvert = 1.648$ amu$^{1/2}$ Å
$\mathcal{S}_1 = 5.784$	$\mathcal{S}_1 = 2.057$
	
$\nu_3(a) = 82$ cm^{-1}	$\nu_4(a) = 157$ cm^{-1}
$\lvert Q_1 \rvert = 5.228$ amu$^{1/2}$ Å	$\lvert Q_1 \rvert = 0.399$ amu$^{1/2}$ Å
$\mathcal{S}_1 = 33.169$	$\mathcal{S}_1 = 0.370$

To be continued ...

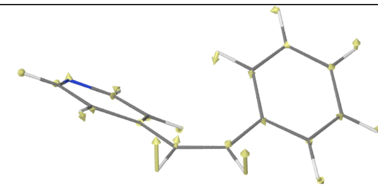
Table S3: *continued.*



$\nu_5(a) = 163$ cm^{-1}

$|Q_1| = 1.700$ amu$^{1/2}$ Å

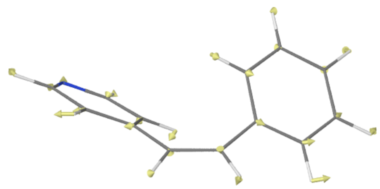
$\mathcal{S}_1 = 6.970$



$\nu_6(a) = 247$ cm^{-1}

$|Q_1| = 0.033$ amu$^{1/2}$ Å

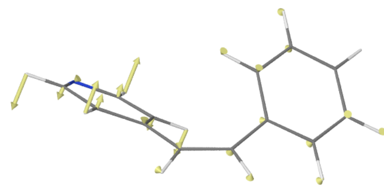
$\mathcal{S}_1 = 0.004$



$\nu_7(a) = 266$ cm^{-1}

$|Q_1| = 0.254$ amu$^{1/2}$ Å

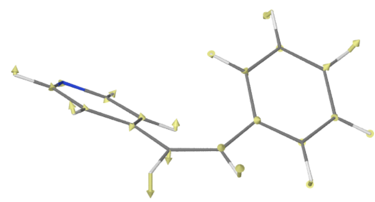
$\mathcal{S}_1 = 0.254$



$\nu_8(a) = 391$ cm^{-1}

$|Q_1| = 0.112$ amu$^{1/2}$ Å

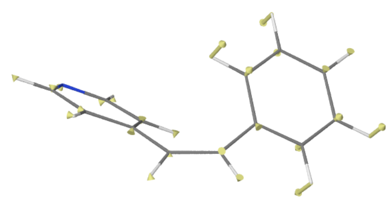
$\mathcal{S}_1 = 0.073$



$\nu_9(a) = 408$ cm^{-1}

$|Q_1| = 0.580$ amu$^{1/2}$ Å

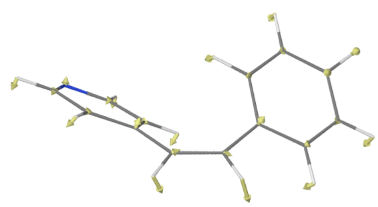
$\mathcal{S}_1 = 2.033$



$\nu_{10}(a) = 413$ cm^{-1}

$|Q_1| = 0.071$ amu$^{1/2}$ Å

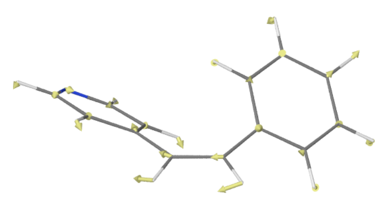
$\mathcal{S}_1 = 0.030$



$\nu_{11}(a) = 464$ cm^{-1}

$|Q_1| = 0.086$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.051$



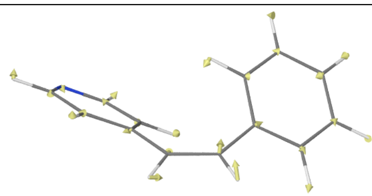
$\nu_{12}(a) = 507$ cm^{-1}

$|Q_1| = 0.081$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.049$

To be continued ...

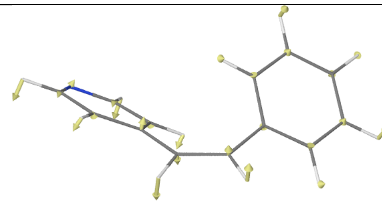
Table S3: *continued.*



$\nu_{13}(a) = 523$ cm^{-1}

$|Q_1| = 0.073$ amu$^{1/2}$ Å

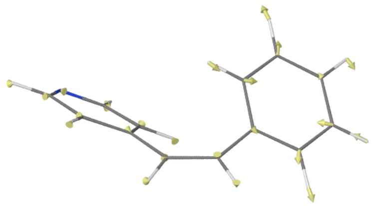
$\mathcal{S}_1 = 0.042$



$\nu_{14}(a) = 584$ cm^{-1}

$|Q_1| = 0.198$ amu$^{1/2}$ Å

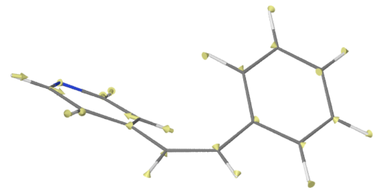
$\mathcal{S}_1 = 0.341$



$\nu_{15}(a) = 623$ cm^{-1}

$|Q_1| = 0.086$ amu$^{1/2}$ Å

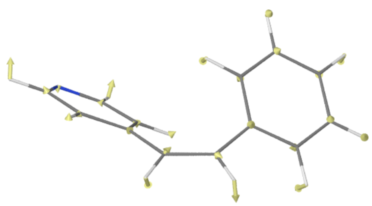
$\mathcal{S}_1 = 0.069$



$\nu_{16}(a) = 674$ cm^{-1}

$|Q_1| = 0.184$ amu$^{1/2}$ Å

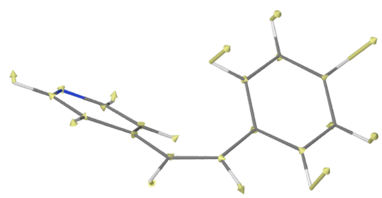
$\mathcal{S}_1 = 0.337$



$\nu_{17}(a) = 701$ cm^{-1}

$|Q_1| = 0.044$ amu$^{1/2}$ Å

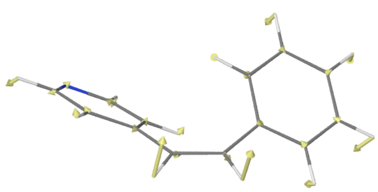
$\mathcal{S}_1 = 0.020$



$\nu_{18}(a) = 712$ cm^{-1}

$|Q_1| = 0.091$ amu$^{1/2}$ Å

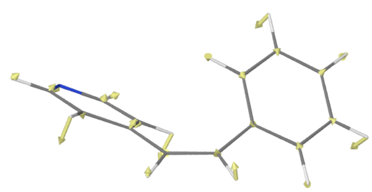
$\mathcal{S}_1 = 0.088$



$\nu_{19}(a) = 747$ cm^{-1}

$|Q_1| = 0.043$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.021$



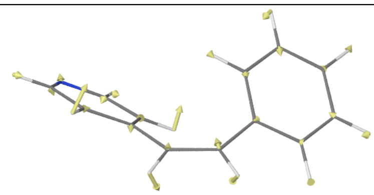
$\nu_{20}(a) = 761$ cm^{-1}

$|Q_1| = 0.092$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.095$

To be continued …

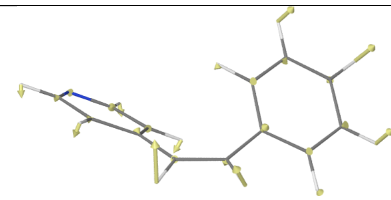
Table S3: *continued.*



$\nu_{21}(a) = 774\ \text{cm}^{-1}$

$|Q_1| = 0.034\ \text{amu}^{1/2}\ \text{Å}$

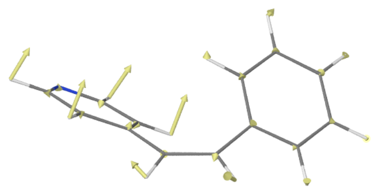
$\mathcal{S}_1 = 0.013$



$\nu_{22}(a) = 798\ \text{cm}^{-1}$

$|Q_1| = 0.188\ \text{amu}^{1/2}\ \text{Å}$

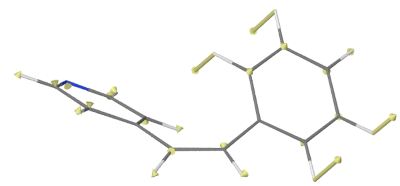
$\mathcal{S}_1 = 0.419$



$\nu_{23}(a) = 837\ \text{cm}^{-1}$

$|Q_1| = 0.196\ \text{amu}^{1/2}\ \text{Å}$

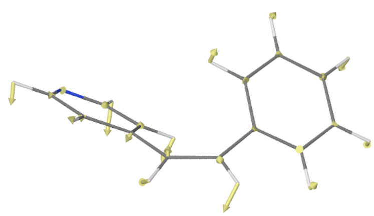
$\mathcal{S}_1 = 0.475$



$\nu_{24}(a) = 862\ \text{cm}^{-1}$

$|Q_1| = 0.186\ \text{amu}^{1/2}\ \text{Å}$

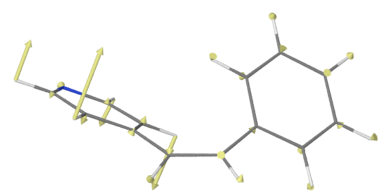
$\mathcal{S}_1 = 0.443$



$\nu_{25}(a) = 891\ \text{cm}^{-1}$

$|Q_1| = 0.394\ \text{amu}^{1/2}\ \text{Å}$

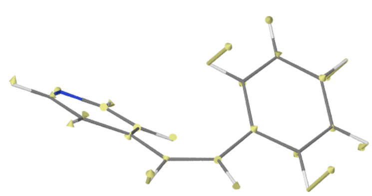
$\mathcal{S}_1 = 2.048$



$\nu_{26}(a) = 892\ \text{cm}^{-1}$

$|Q_1| = 0.241\ \text{amu}^{1/2}\ \text{Å}$

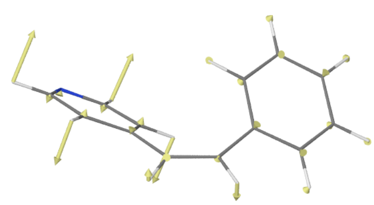
$\mathcal{S}_1 = 0.768$



$\nu_{27}(a) = 941\ \text{cm}^{-1}$

$|Q_1| = 0.201\ \text{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0.563$



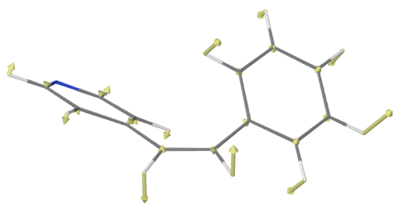
$\nu_{28}(a) = 976\ \text{cm}^{-1}$

$|Q_1| = 0.202\ \text{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0.592$

To be continued …

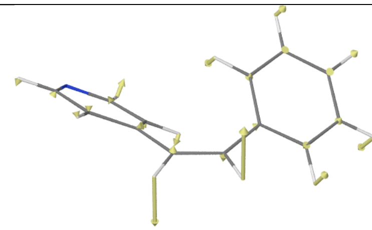
Table S3: *continued.*



$\nu_{29}(a) = 988\ \mathrm{cm}^{-1}$

$|Q_1| = 0.102\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

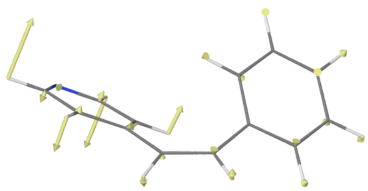
$\mathcal{S}_1 = 0.153$



$\nu_{30}(a) = 989\ \mathrm{cm}^{-1}$

$|Q_1| = 0.152\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

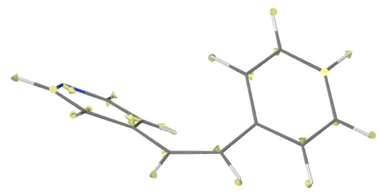
$\mathcal{S}_1 = 0.338$



$\nu_{31}(a) = 995\ \mathrm{cm}^{-1}$

$|Q_1| = 0.161\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

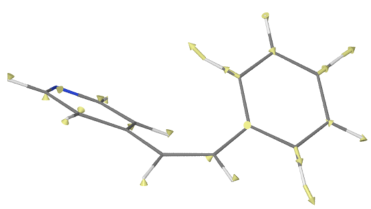
$\mathcal{S}_1 = 0.382$



$\nu_{32}(a) = 1001\ \mathrm{cm}^{-1}$

$|Q_1| = 0.188\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

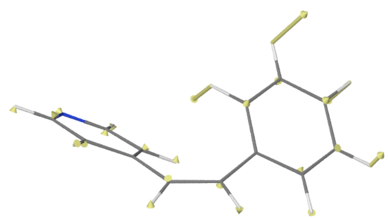
$\mathcal{S}_1 = 0.526$



$\nu_{33}(a) = 1005\ \mathrm{cm}^{-1}$

$|Q_1| = 0.056\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

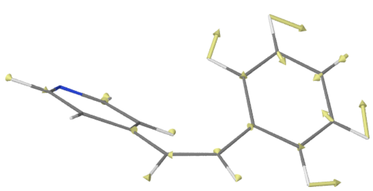
$\mathcal{S}_1 = 0.047$



$\nu_{34}(a) = 1008\ \mathrm{cm}^{-1}$

$|Q_1| = 0.169\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

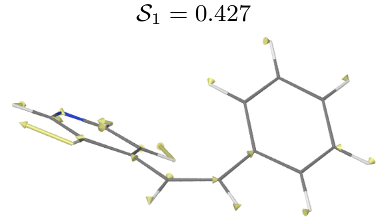
$\mathcal{S}_1 = 0.427$



$\nu_{35}(a) = 1045\ \mathrm{cm}^{-1}$

$|Q_1| = 0.187\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

$\mathcal{S}_1 = 0.547$



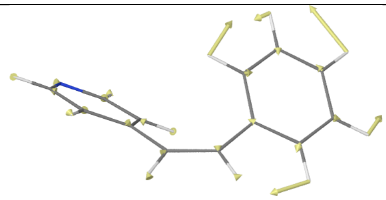
$\nu_{36}(a) = 1089\ \mathrm{cm}^{-1}$

$|Q_1| = 0.199\ \mathrm{amu}^{1/2}\ \mathrm{Å}$

$\mathcal{S}_1 = 0.636$

To be continued ...

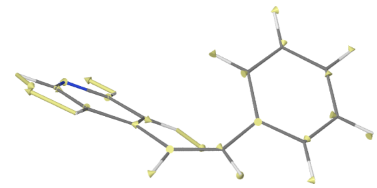
Table S3: *continued.*



$\nu_{37}(a) = 1101$ cm^{-1}

$|Q_1| = 0.043$ amu$^{1/2}$ Å

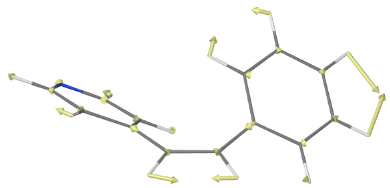
$\mathcal{S}_1 = 0.031$



$\nu_{38}(a) = 1113$ cm^{-1}

$|Q_1| = 0.065$ amu$^{1/2}$ Å

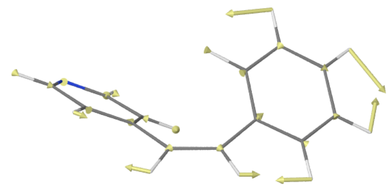
$\mathcal{S}_1 = 0.071$



$\nu_{39}(a) = 1177$ cm^{-1}

$|Q_1| = 0.10$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.002$



$\nu_{40}(a) = 1180$ cm^{-1}

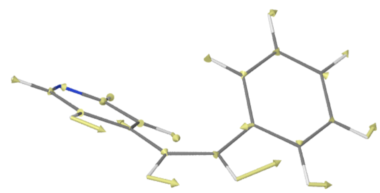
$|Q_1| = 0.011$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.002$

$\nu_{41}(a) = 1201$ cm^{-1}

$|Q_1| = 0.088$ amu$^{1/2}$ Å

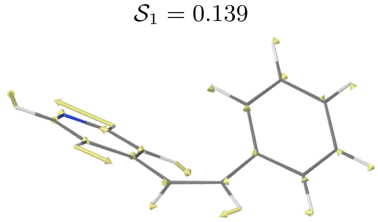
$\mathcal{S}_1 = 0.139$



$\nu_{42}(a) = 1229$ cm^{-1}

$|Q_1| = 0.000$ amu$^{1/2}$ Å

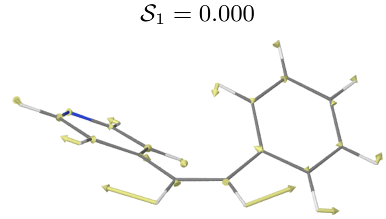
$\mathcal{S}_1 = 0.000$



$\nu_{43}(a) = 1244$ cm^{-1}

$|Q_1| = 0.035$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.022$



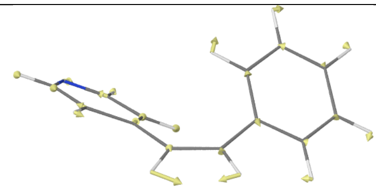
$\nu_{44}(a) = 1261$ cm^{-1}

$|Q_1| = 0.005$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.000$

To be continued ...

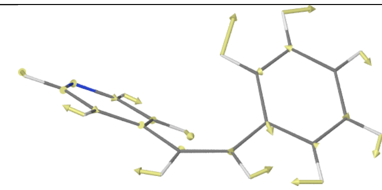
Table S3: *continued.*



$\nu_{45}(a) = 1311$ cm^{-1}

$|Q_1| = 0.010$ amu$^{1/2}$ Å

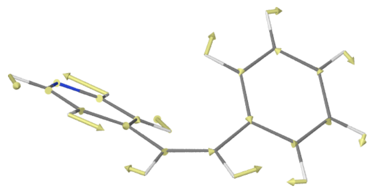
$\mathcal{S}_1 = 002$



$\nu_{46}(a) = 1344$ cm^{-1}

$|Q_1| = 0.022$ amu$^{1/2}$ Å

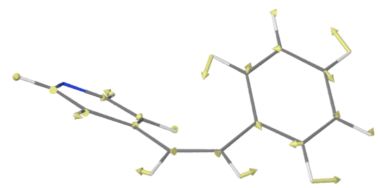
$\mathcal{S}_1 = 0.010$



$\nu_{47}(a) = 1358$ cm^{-1}

$|Q_1| = 0.113$ amu$^{1/2}$ Å

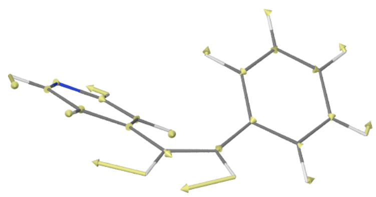
$\mathcal{S}_1 = 0.259$



$\nu_{48}(a) = 1362$ cm^{-1}

$|Q_1| = 0.047$ amu$^{1/2}$ Å

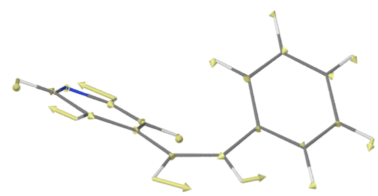
$\mathcal{S}_1 = 0.045$



$\nu_{49}(a) = 1432$ cm^{-1}

$|Q_1| = 0.101$ amu$^{1/2}$ Å

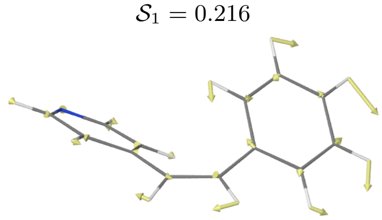
$\mathcal{S}_1 = 0.216$



$\nu_{50}(a) = 1446$ cm^{-1}

$|Q_1| = 0.125$ amu$^{1/2}$ Å

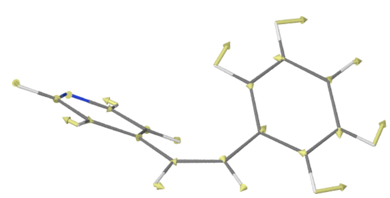
$\mathcal{S}_1 = 0.333$



$\nu_{51}(a) = 1471$ cm^{-1}

$|Q_1| = 0.078$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.134$



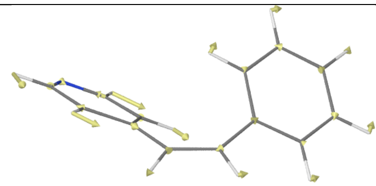
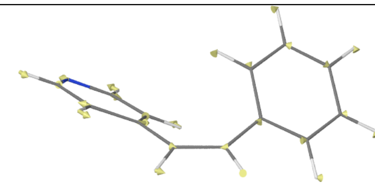
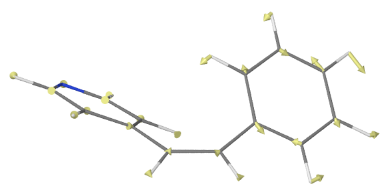
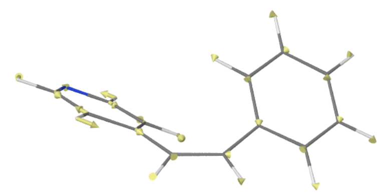
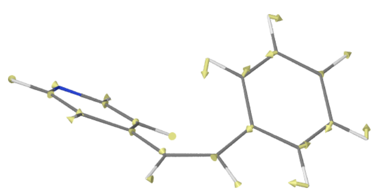
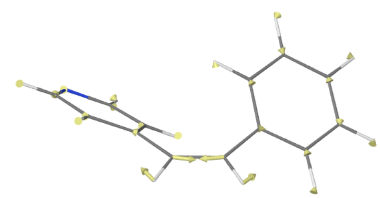
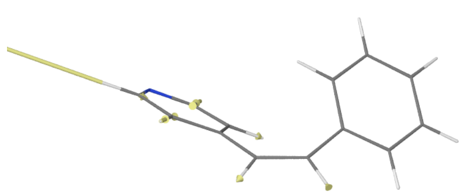
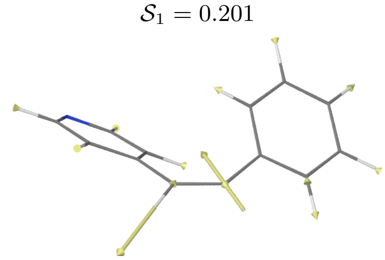
$\nu_{52}(a) = 1515$ cm^{-1}

$|Q_1| = 0.037$ amu$^{1/2}$ Å

$\mathcal{S}_1 = 0.032$

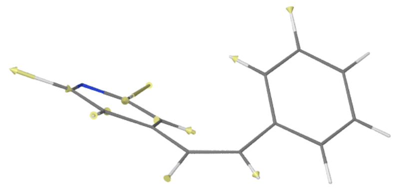
To be continued ...

Table S3: *continued.*

 $\nu_{53}(a) = 1525$ cm^{-1} $\lvert Q_1 \rvert = 0.242$ amu$^{1/2}$ Å $\mathcal{S}_1 = 1.322$	 $\nu_{54}(a) = 1596$ cm^{-1} $\lvert Q_1 \rvert = 0.034$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.028$
 $\nu_{55}(a) = 1618$ cm^{-1} $\lvert Q_1 \rvert = 0.057$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.077$	 $\nu_{56}(a) = 1637$ cm^{-1} $\lvert Q_1 \rvert = 0.030$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.021$
 $\nu_{57}(a) = 1647$ cm^{-1} $\lvert Q_1 \rvert = 0.021$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.011$	 $\nu_{58}(a) = 1682$ cm^{-1} $\lvert Q_1 \rvert = 0.090$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.201$
 $\nu_{59}(a) = 3158$ cm^{-1} $\lvert Q_1 \rvert = 0.006$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.001$	 $\nu_{60}(a) = 3164$ cm^{-1} $\lvert Q_1 \rvert = 0.002$ amu$^{1/2}$ Å $\mathcal{S}_1 = 0.000$

To be continued ...

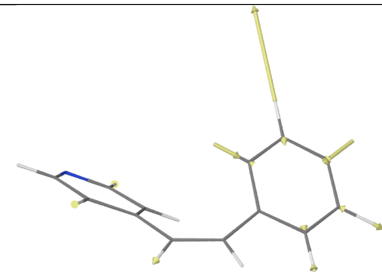
Table S3: *continued.*



$\nu_{61}(a) = 3165\ \mathrm{cm}^{-1}$

$|Q_1| = 0.028\ \mathrm{amu}^{1/2}$ Å

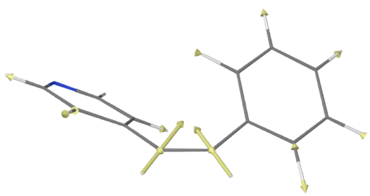
$\mathcal{S}_1 = 0.036$



$\nu_{62}(a) = 3181\ \mathrm{cm}^{-1}$

$|Q_1| = 0.020\ \mathrm{amu}^{1/2}$ Å

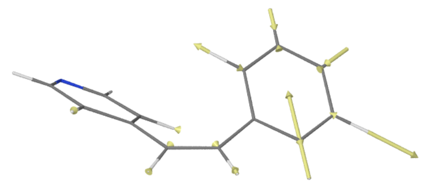
$\mathcal{S}_1 = 0.019$



$\nu_{63}(a) = 3185\ \mathrm{cm}^{-1}$

$|Q_1| = 0.013\ \mathrm{amu}^{1/2}$ Å

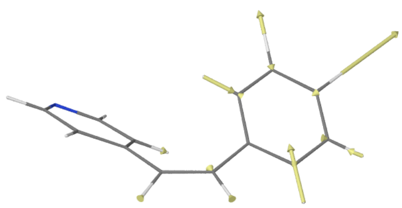
$\mathcal{S}_1 = 0.008$



$\nu_{64}(a) = 3195\ \mathrm{cm}^{-1}$

$|Q_1| = 0.012\ \mathrm{amu}^{1/2}$ Å

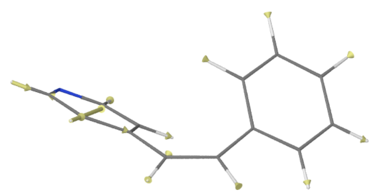
$\mathcal{S}_1 = 0.007$



$\nu_{65}(a) = 3202\ \mathrm{cm}^{-1}$

$|Q_1| = 0.020\ \mathrm{amu}^{1/2}$ Å

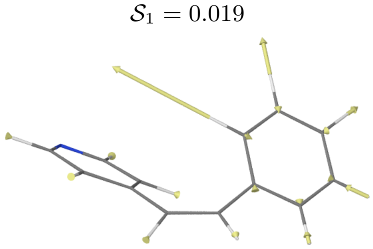
$\mathcal{S}_1 = 0.019$



$\nu_{66}(a) = 3208\ \mathrm{cm}^{-1}$

$|Q_1| = 0.044\ \mathrm{amu}^{1/2}$ Å

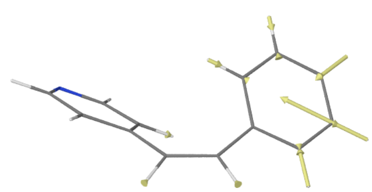
$\mathcal{S}_1 = 0.094$



$\nu_{67}(a) = 3210\ \mathrm{cm}^{-1}$

$|Q_1| = 0.087\ \mathrm{amu}^{1/2}$ Å

$\mathcal{S}_1 = 0.363$



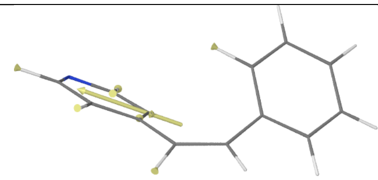
$\nu_{68}(a) = 3221\ \mathrm{cm}^{-1}$

$|Q_1| = 0.048\ \mathrm{amu}^{1/2}$ Å

$\mathcal{S}_1 = 0.108$

To be continued ...

Table S3: *continued.*



$\nu_{69}(a) = 3242\ \mathrm{cm}^{-1}$

$|Q_1| = 0.086\ \mathrm{amu}^{1/2}\ \text{Å}$

$\mathcal{S}_1 = 0.354$