Supporting Information for "Excitonic Splitting and Vibronic Coupling Analysis of the *meta*-Cyanophenol Dimer"

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Figure S1: C_2-symmetric, stacked structure of the meta-cyanophenol dimer, calculated with the SCS-CC2/aVTZ method.

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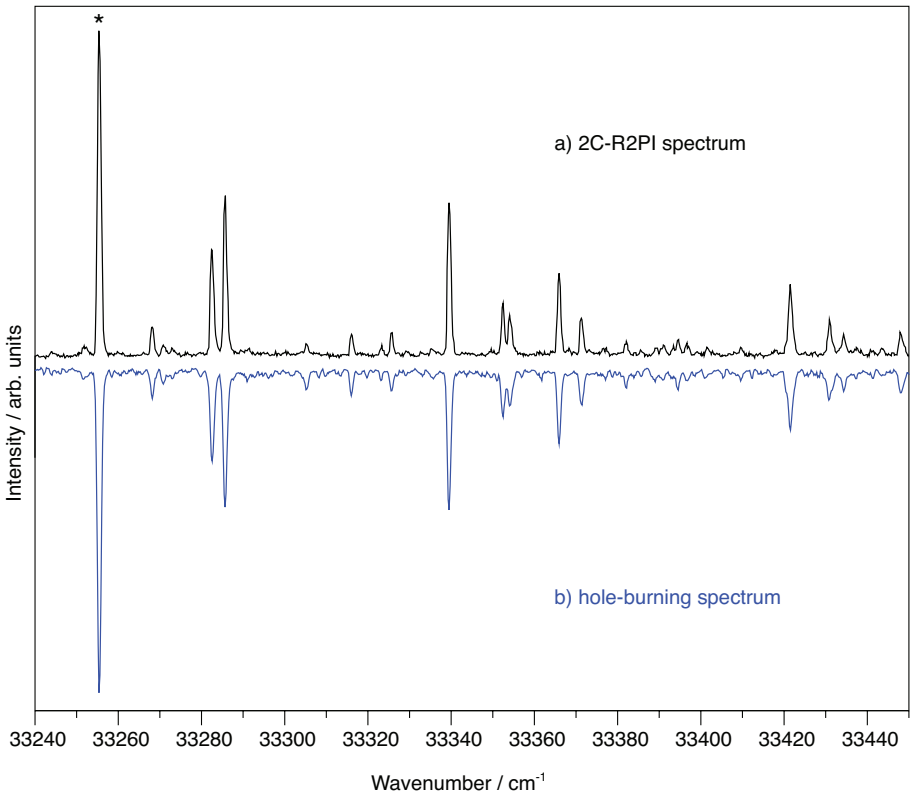

Figure S2: (a) Two-color R2PI spectrum of supersonic jet-cooled (m-cyanophenol)$_2$, cf. Figure 8(a) of the main paper. The UV holeburning laser is then positioned at the center of the 0_0^0 band, marked by an asterisk. The depletion of the 0_0^0 band R2PI signal is maximized, and the R2PI spectrum is remeasured, giving the holeburned spectrum (b), which is the difference of the R2PI spectra without and with holeburning laser, plotted downwards for comparison with (a). The intensity of the 0_0^0 band of the holeburned spectrum is scaled to match that of the 0_0^0 band in (a).

Table S1: Cartesian coordinates of the SCS-CC2/aVTZ optimized, z-shaped, C_i-symmetric *meta*-cyanophenol dimer.

Atom	x	y	z
C	-0.606881	-1.890326	-0.041769
C	-1.747352	-2.696816	-0.054901
C	-1.601110	-4.092254	-0.031475
C	-0.330547	-4.664167	0.007100
C	0.820264	-3.871276	0.026132
C	0.664069	-2.481607	0.000985
O	-3.004316	-2.189627	-0.090258
C	1.793904	-1.593346	0.024056
N	2.646763	-0.783980	0.045138
O	3.004316	2.189627	0.090258
C	1.747352	2.696816	0.054901
C	0.606881	1.890326	0.041769
C	-0.664069	2.481607	-0.000985
C	-0.820264	3.871276	-0.026132
C	0.330547	4.664167	-0.007100
C	1.601110	4.092254	0.031475
C	-1.793904	1.593346	-0.024056
N	-2.646763	0.783980	-0.045138
H	-2.490626	-4.709097	-0.043121
H	-0.235936	-5.742483	0.024448
H	1.806944	-4.312797	0.059850
H	-0.708928	-0.816162	-0.064753
H	-2.973694	-1.214122	-0.084731
H	0.708928	0.816162	0.064753
H	2.973694	1.214122	0.084731
H	2.490626	4.709097	0.043121
H	0.235936	5.742483	-0.024448
H	-1.806944	4.312797	-0.059850

Table S2: Cartesian coordinates of the SCS-CC2/aVTZ optimized, planar, C_{2h}-symmetric *meta*-cyanophenol dimer.

Atom	x	y	z
C	-0.602702	-1.855402	0.000000
C	-1.752877	-2.670145	0.000000
C	-1.607959	-4.077211	0.000000
C	-0.326256	-4.656188	0.000000
C	0.835677	-3.859551	0.000000
C	0.677665	-2.456727	0.000000
O	-3.019807	-2.162432	0.000000
C	1.814197	-1.568098	0.000000
N	2.688637	-0.751544	0.000000
O	3.019807	2.162432	0.000000
C	1.752877	2.670145	0.000000
C	0.602702	1.855402	0.000000
C	-0.677665	2.456727	0.000000
C	-0.835677	3.859551	0.000000
C	0.326256	4.656188	0.000000
C	1.607959	4.077211	0.000000
C	-1.814197	1.568098	0.000000
N	-2.688637	0.751544	0.000000
H	-2.508876	-4.697298	0.000000
H	-0.232118	-5.746054	0.000000
H	1.833180	-4.305451	0.000000
H	-0.703585	-0.769670	0.000000
H	-2.986488	-1.179123	0.000000
H	0.703585	0.769670	0.000000
H	2.986488	1.179123	0.000000
H	2.508876	4.697298	0.000000
H	0.232118	5.746054	0.000000
H	-1.833180	4.305451	0.000000

Table S3: Cartesian coordinates of the SCS-CC2/aVTZ optimized, V-shaped, C_2-symmetric *meta*-cyanophenol dimer.

Atom	x	y	z
C	-0.154715	-1.979385	-0.055577
C	-1.078303	-3.026175	-0.005552
C	-0.613689	-4.347490	0.080560
C	0.754902	-4.609100	0.118179
C	1.691741	-3.572844	0.074503
C	1.218762	-2.259500	-0.012886
O	-2.418704	-2.824180	-0.037108
C	2.113295	-1.135209	-0.055876
N	2.756651	-0.151455	-0.090748
O	2.418704	2.824180	-0.037108
C	1.078303	3.026175	-0.005552
C	0.154715	1.979385	-0.055577
C	-1.218762	2.259500	-0.012886
C	-1.691741	3.572844	0.074503
C	-0.754902	4.609100	0.118179
C	0.613689	4.347490	0.080560
C	-2.113295	1.135209	-0.055876
N	-2.756651	0.151455	-0.090748
H	-1.336884	-5.152149	0.117748
H	1.096032	-5.634407	0.184426
H	2.753985	-3.773257	0.107400
H	-0.502258	-0.960035	-0.125700
H	-2.614091	-1.868578	-0.072010
H	0.502258	0.960035	-0.125700
H	2.614091	1.868578	-0.072010
H	1.336884	5.152149	0.117748
H	-1.096032	5.634407	0.184426
H	-2.753985	3.773257	0.107400

Table S4: Cartesian coordinates of the SCS-CC2/aVTZ optimized, stacked C_2-symmetric *meta*-cyanophenol dimer.

Atom	x	y	z
C	-1.867457	-2.646361	0.989844
C	-1.976603	-1.874684	-0.176765
C	-0.828346	-1.565447	-0.911568
C	0.421906	-2.002588	-0.447265
C	0.542940	-2.761059	0.722793
C	-0.622401	-3.112421	1.409671
O	-3.221369	-1.458193	-0.535945
C	1.591303	-1.583526	-1.170956
N	2.512541	-1.143588	-1.757210
O	3.221369	1.458193	-0.535945
C	1.976603	1.874684	-0.176765
C	1.867457	2.646361	0.989844
C	0.622401	3.112421	1.409671
C	-0.542940	2.761059	0.722793
C	-0.421906	2.002588	-0.447265
C	0.828346	1.565447	-0.911568
C	-1.591303	1.583526	-1.170956
N	-2.512541	1.143588	-1.757210
H	-2.766739	-2.872320	1.548668
H	-0.556965	-3.732027	2.295223
H	1.517586	-3.073930	1.072598
H	-0.899039	-0.994585	-1.828195
H	-3.152206	-0.759807	-1.210893
H	0.899039	0.994585	-1.828195
H	3.152206	0.759807	-1.210893
H	2.766739	2.872320	1.548668
H	0.556965	3.732027	2.295223
H	-1.517586	3.073930	1.072598