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Conformationally resolved structures of jet-cooled acetaminophen by UV-UV hole-burning spectroscopy

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Figure S1

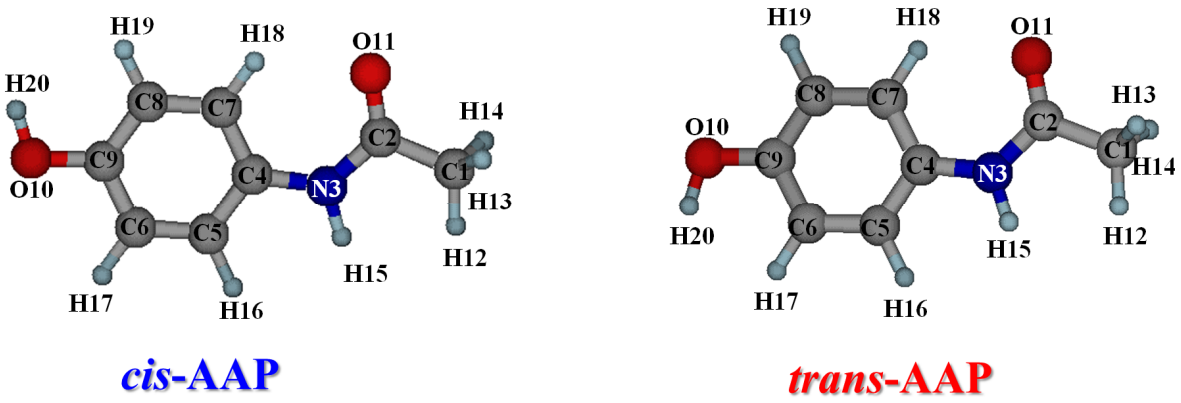

Table S1

(a) Optimized structure of *cis*-AAP by B3LYP/aug-cc-pVDZ

Atomic Number	Coordinates (Å)		
	X	Y	Z
C1	-1.365895	-0.006289	-3.766351
C2	-1.365762	-0.007352	-2.246732
N3	-0.117072	-0.007177	-1.670171
C4	0.233858	-0.002352	-0.298413
C5	1.602934	-0.003488	0.020338
C6	2.034815	0.001187	1.343663
C7	-0.705515	0.00345	0.74361
C8	-0.268852	0.008104	2.071749
C9	1.094372	0.007047	2.379532
O10	1.572323	0.011458	3.667829
O11	-2.411832	-0.00554	-1.608015
H12	-0.36323	-0.038911	-4.211429
H13	-1.883102	0.897405	-4.114307
H14	-1.94298	-0.872076	-4.115204

H15	0.665082	-0.009711	-2.308979
H16	2.346013	-0.007958	-0.779701
H17	3.096756	0.000286	1.585343
H18	-1.76518	0.004166	0.511581
H19	-1.009839	0.012594	2.873934
H20	0.832316	0.015258	4.287067

(b) Optimized structure of *trans*-AAP by B3LYP/aug-cc-pVDZ

Atomic Number	Coordinates (Å)		
	X	Y	Z
C1	-1.401345	-0.00651	-3.753809
C2	-1.390024	-0.00655	-2.234059
N3	-0.136325	-0.006884	-1.667436
C4	0.227142	-0.002274	-0.298804
C5	1.596375	-0.00403	0.007736
C6	2.035467	0.000389	1.331966
C7	-0.704918	0.003922	0.753389
C8	-0.262883	0.008318	2.076639
C9	1.102823	0.006601	2.374624
O10	1.466364	0.011154	3.699952
O11	-2.431097	-0.004047	-1.588008
H12	-0.402013	-0.035406	-4.206638
H13	-1.924981	0.894731	-4.098379
H14	-1.977505	-0.874911	-4.097724
H15	0.639861	-0.009971	-2.313394
H16	2.334905	-0.008822	-0.796432
H17	3.105752	-0.001051	1.547513
H18	-1.765963	0.005156	0.527894
H19	-0.982128	0.013121	2.894779
H20	2.428396	0.009299	3.772781

Table S2

AAP	Method Basis set	Energy (Hartree)	Relative Energy (kJ/mol)	Dipole moment (D)	Rotational constants (GHz)	
cis-	B3LYP aug-cc-pVDZ	-515.4001	0	2.30	A	3.60164
					B	0.54143
					C	0.47206
trans-	B3LYP aug-cc-pVDZ	-515.3996	1.37	4.77	A	3.59636
					B	0.54161
					C	0.47211
cis-	MP2 aug-cc-pVDZ	-513.9441	0	2.24	A	3.55707
					B	0.53997
					C	0.4702
trans-	MP2 aug-cc-pVDZ	-513.9436	1.41	4.71	A	3.54876
					B	0.54024
					C	0.47025

Table S3

cis-AAP				trans-AAP			
Harmonic Freq. (cm^{-1})	Intensity (km/mol)	Harmonic Freq. (cm^{-1})	Intensity (km/mol)	Harmonic Freq. (cm^{-1})	Intensity (km/mol)	Harmonic Freq. (cm^{-1})	Intensity (km/mol)
3817.8	72.4	1019.9	4.2	3819.2	73.3	1019.5	4.0
3623.0	19.6	1006.1	13.8	3623.2	18.7	1005.7	15.2
3254.2	7.4	989.0	1.1	3255.0	7.5	1003.9	0.5
3203.2	4.4	967.5	0.0	3199.4	4.0	963.6	3.7
3164.4	2.9	962.8	0.8	3174.1	11.8	945.9	0.1
3162.5	27.2	865.0	5.2	3157.7	18.7	864.9	43.0
3127.7	8.4	853.1	58.7	3127.4	7.7	863.0	3.9

3124.1	**12.1**	**820.6**	**1.4**	**3124.2**	**13.0**	**809.2**	**18.8**
3044.3	**11.2**	**797.9**	**19.9**	**3044.2**	**11.3**	**797.0**	**24.0**
1732.3	**252.6**	**740.2**	**0.0**	**1734.0**	**257.1**	**738.5**	**0.0**
1659.9	**9.9**	**653.2**	**0.0**	**1662.7**	**2.0**	**653.3**	**1.8**
1644.5	**6.5**	**627.8**	**8.2**	**1639.8**	**38.4**	**627.3**	**4.4**
1554.7	**379.2**	**626.1**	**3.3**	**1557.5**	**403.1**	**626.0**	**6.4**
1536.2	**266.4**	**550.4**	**39.0**	**1531.8**	**104.5**	**549.0**	**38.6**
1465.4	**6.7**	**529.8**	**31.0**	**1465.9**	**37.8**	**529.1**	**31.8**
1446.6	**27.4**	**503.9**	**24.8**	**1449.4**	**134.0**	**503.7**	**26.0**
1443.9	**7.6**	**428.4**	**0.3**	**1443.8**	**7.3**	**427.7**	**0.7**
1379.2	**29.2**	**425.6**	**9.2**	**1378.8**	**66.8**	**425.1**	**7.4**
1370.3	**13.6**	**381.8**	**0.2**	**1370.1**	**45.0**	**381.3**	**0.1**
1334.5	**70.9**	**354.2**	**96.3**	**1330.0**	**23.0**	**338.4**	**95.3**
1282.0	**20.6**	**325.3**	**1.0**	**1283.3**	**20.0**	**324.2**	**3.3**
1253.6	**216.0**	**312.1**	**0.0**	**1255.1**	**170.9**	**312.5**	**4.9**
1235.9	**15.5**	**188.4**	**0.0**	**1234.7**	**16.6**	**187.8**	**0.0**
1189.7	**103.7**	**153.6**	**8.9**	**1187.8**	**184.3**	**153.8**	**4.1**
1182.9	**70.2**	**81.5**	**1.5**	**1186.4**	**1.1**	**81.1**	**1.3**
1124.6	**26.3**	**52.8**	**7.7**	**1125.8**	**11.3**	**50.6**	**2.8**
1035.1	**4.8**	**39.3**	**1.6**	**1034.8**	**4.8**	**38.6**	**1.7**