

Infrared Spectrum and UV-Induced Photochemistry of Matrix-Isolated Phenyl 1-Hydroxy-2-Naphthoate

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Supporting Information

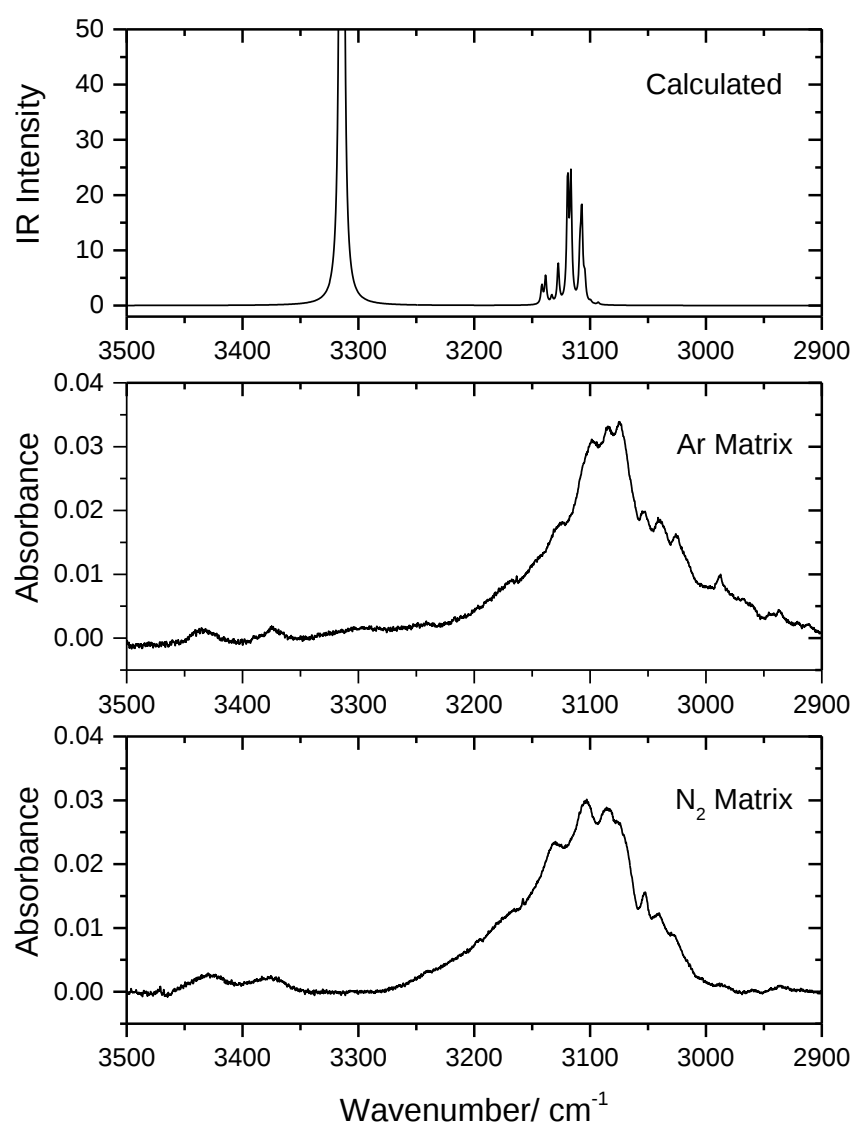


Figure S1. Infrared spectrum of PHN in Ar (*middle panel*) and N₂ (*bottom*) matrices (10 K) and B3LYP/6-311++G(d,p) calculated spectrum for PHN conformer **1** (*top*) in the 3500-2900 cm⁻¹ range. In the calculated spectrum, wavenumbers are scaled by 0.978.

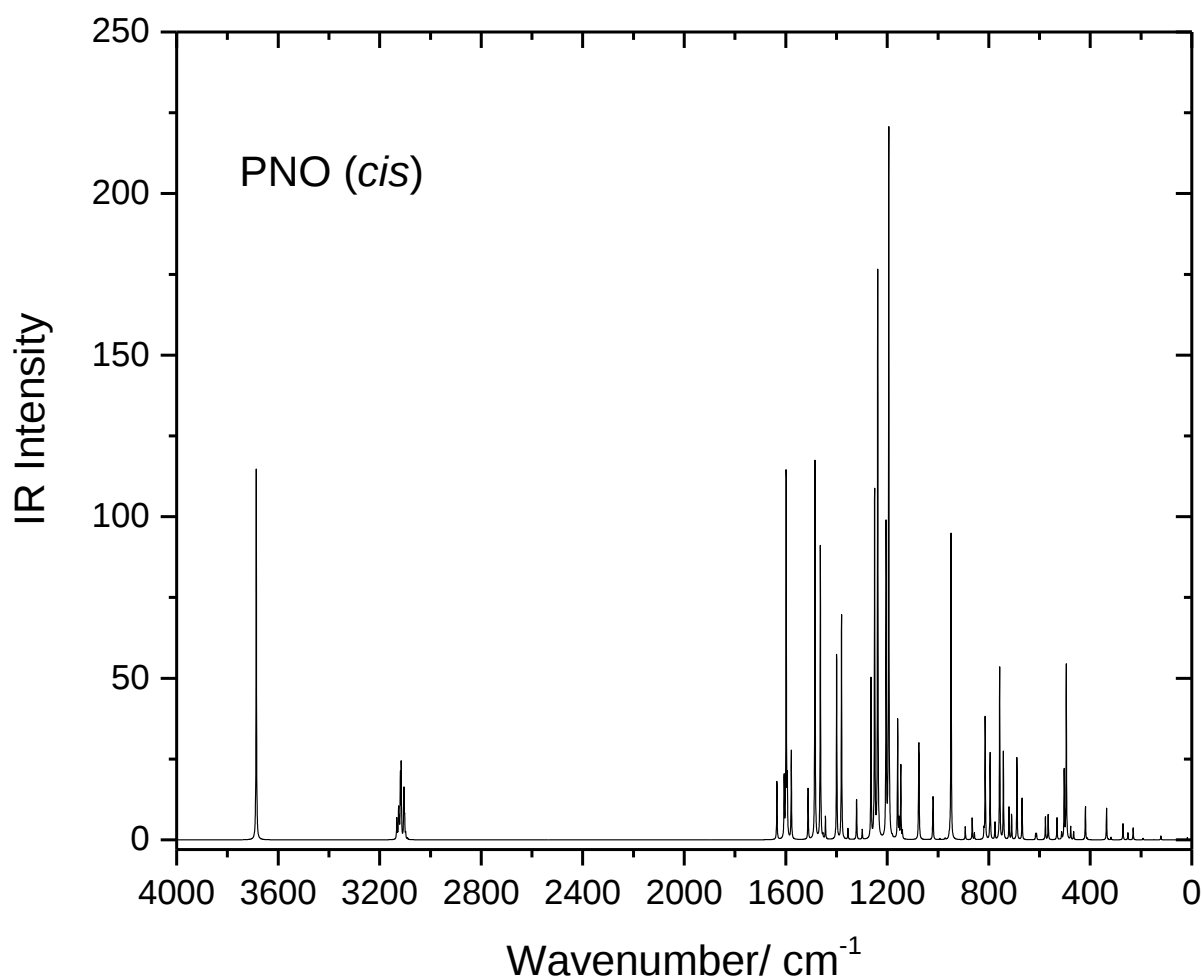


Figure S2. B3LYP/6-311++G(d,p) calculated spectrum for PNO conformer *cis*. Wavenumbers are scaled by 0.978.

Table S1. UV-irradiation parameters of PHN in Ar and N₂ matrices.

Ar Matrix			N ₂ Matrix		
Wavelength	Pulse energy	Exposure time	Wavelength	Pulse energy	Exposure time
331.7 nm	20 mW	15 min	331.7 nm	5 mW	30 min
278.0 nm	14 mW	2 min	276.0 nm	3 mW	6 min
265.0 nm	27 mW	2 min	265.0 nm	8 mW	5 min
250.0 nm	17 mW	2 min	250.0 nm	3 mW	15 min
235.0 nm	5 mW	2 min			

Table S2. Optimized Cartesian coordinates (in Å) for the conformers of PHN.

Atomic Number	X	Y	Z	Atomic number	X	Y	Z
Conformer 1				Conformer 2			
6	5.895622000	0.069324000	0.003342000	6	4.749254000	-1.725482000	-0.151678000
6	5.128037000	0.567568000	1.055814000	6	5.477098000	-0.519952000	-0.052697000
6	3.751802000	0.355213000	1.087513000	6	4.818023000	0.683917000	0.050278000
6	3.159790000	-0.355806000	0.050990000	6	3.402592000	0.740351000	0.059228000
6	3.906169000	-0.861365000	-1.004845000	6	2.671953000	-0.479758000	-0.041006000
6	5.283315000	-0.645559000	-1.024235000	6	3.373034000	-1.706601000	-0.145921000
8	1.791587000	-0.662320000	0.083386000	6	2.694636000	1.971645000	0.164830000
6	0.879822000	0.336415000	-0.045452000	6	1.331338000	1.982613000	0.169354000
6	-0.504653000	-0.131854000	0.018520000	6	0.569312000	0.779700000	0.070296000
6	-0.830126000	-1.507348000	0.208401000	6	1.239431000	-0.443378000	-0.033756000
6	-2.127724000	-1.925813000	0.264046000	8	0.630641000	-1.132147000	-0.132147000
6	-3.196239000	-0.990976000	0.132066000	6	-0.895733000	0.946879000	0.087557000
6	-2.902653000	0.391372000	-0.057873000	8	-1.572623000	-0.271450000	-0.007588000
6	-1.534636000	0.809525000	-0.112824000	6	-2.978417000	-0.268578000	-0.017246000
6	-4.554485000	-1.389563000	0.183171000	8	-1.489505000	1.987748000	0.173285000
6	-5.567627000	-0.466406000	0.053163000	6	-3.661478000	0.097172000	-1.169514000
6	-5.270060000	0.900804000	-0.133948000	6	-5.052501000	0.024636000	-1.176873000
6	-3.960942000	1.322817000	-0.188573000	6	-5.740909000	-0.412717000	-0.045475000
8	1.210799000	1.504096000	-0.203666000	6	-5.036026000	-0.776679000	1.100302000
8	-1.306962000	2.116704000	-0.292697000	6	-3.643963000	-0.703660000	1.120293000
1	6.966167000	0.236982000	-0.014363000	1	5.278017000	-2.668213000	-0.232747000
1	5.600198000	1.123550000	1.857557000	1	6.561149000	-0.545293000	-0.058059000
1	3.146237000	0.737576000	1.899247000	1	5.376658000	1.610585000	0.126753000
1	3.409830000	-1.415525000	-1.792121000	1	2.807567000	-2.625761000	-0.221635000
1	5.874612000	-1.037272000	-1.843822000	1	3.252885000	2.897624000	0.241516000
1	-0.018225000	-2.214894000	0.309261000	1	0.780144000	2.910802000	0.249180000
1	-2.361198000	-2.974319000	0.409324000	1	-0.333103000	-1.503877000	-0.119000000
1	-4.784768000	-2.439718000	0.327340000	1	-3.112582000	0.435893000	-2.039299000
1	-6.602029000	-0.789235000	0.094510000	1	-5.597605000	0.309732000	-2.069115000
1	-6.076326000	1.618115000	-0.234988000	1	-6.823136000	-0.468705000	-0.057382000
1	-3.719893000	2.367931000	-0.332256000	1	-5.566653000	-1.116716000	1.982043000
1	-0.330472000	2.248880000	-0.311520000	1	-3.077301000	-0.979036000	2.001517000
Conformer 3				Conformer 4			
6	4.853498000	-0.309050000	0.664791000	6	5.916907000	-0.036669000	0.000965000
6	4.685364000	-1.622805000	0.177256000	6	5.284600000	-0.625241000	1.094443000
6	3.474776000	-2.025900000	-0.341050000	6	3.898879000	-0.775370000	1.106321000
6	2.375205000	-1.135725000	-0.394672000	6	3.157911000	-0.336195000	0.015462000
6	2.550878000	0.189011000	0.100754000	6	3.773438000	0.250343000	-1.085590000
6	3.805331000	0.582571000	0.626036000	6	5.158181000	0.399890000	-1.084935000
6	1.112895000	-1.522896000	-0.934196000	8	1.784705000	-0.582698000	0.030638000
6	0.070350000	-0.644713000	-0.960174000	6	0.905572000	0.484121000	-0.027863000
6	0.205242000	0.684687000	-0.456713000	6	-0.496462000	-0.008875000	-0.052615000
6	1.448627000	1.100926000	0.049791000	6	-0.763863000	-1.393032000	-0.249081000
8	1.668190000	2.339651000	0.500900000	6	-2.038460000	-1.884477000	-0.287244000
6	-0.892016000	1.649389000	-0.476357000	6	-3.147757000	-1.013179000	-0.132503000
8	-2.122658000	1.225668000	-0.925495000	6	-2.918830000	0.383698000	0.061823000
8	-0.768075000	2.829116000	-0.188013000	6	-1.568295000	0.868333000	0.110399000
6	-2.861313000	0.273917000	-0.238018000	6	-4.482882000	-1.488907000	-0.168907000
6	-2.719689000	0.064628000	1.131816000	6	-5.548695000	-0.634034000	-0.027359000
6	-3.530100000	-0.880563000	1.759199000	6	-5.325778000	0.748297000	0.151850000
6	-4.479164000	-1.596756000	1.033319000	6	-4.042376000	1.241645000	0.192139000
6	-4.618982000	-1.361917000	-0.334780000	8	1.276521000	1.625684000	-0.055057000
6	-3.811380000	-0.427975000	-0.976965000	8	-1.320264000	2.179854000	0.319177000
1	5.811545000	-0.003441000	1.069026000	1	6.994255000	0.081543000	-0.006126000
1	5.517161000	-2.317657000	0.210807000	1	5.867297000	-0.968009000	1.941900000
1	3.348083000	-3.035495000	-0.716763000	1	3.387495000	-1.229967000	1.946161000
1	3.922162000	1.593449000	0.993978000	1	3.177548000	0.589943000	-1.922809000
1	0.993532000	-2.526940000	-1.324549000	1	5.644547000	0.859356000	-1.937862000
1	-0.880157000	-0.949557000	-1.375530000	1	0.079644000	-2.057815000	-0.368301000
1	0.843597000	2.860603000	0.351492000	1	-2.215282000	-2.943249000	-0.437407000
1	-1.996735000	0.633594000	1.703687000	1	-4.648338000	-2.552170000	-0.313362000
1	-3.420277000	-1.047389000	2.824642000	1	-6.562867000	-1.015590000	-0.057320000
1	-5.108321000	-2.326327000	1.529019000	1	-6.167747000	1.423119000	0.251595000
1	-5.359825000	-1.907927000	-0.907694000	1	-3.918454000	2.313851000	0.312610000
1	-3.907557000	-0.229374000	-2.037476000	1	-2.138334000	2.641017000	0.529040000
Conformer 5				Conformer 6			
6	4.792994000	-1.688599000	0.160681000	6	3.405790000	-2.368444000	0.859391000
6	5.495890000	-0.484908000	-0.060604000	6	2.643254000	-1.537002000	1.678252000
6	4.807443000	0.694558000	-0.214676000	6	2.280340000	-0.261471000	1.250136000
6	3.391436000	0.733432000	-0.149692000	6	2.674038000	0.163867000	-0.016206000
6	2.677306000	-0.481601000	0.087548000	6	3.443672000	-0.650446000	-0.841323000
6	3.419057000	-1.683806000	0.230004000	6	3.808927000	-1.919268000	-0.397704000
6	2.668920000	1.944161000	-0.313681000	8	2.398528000	1.452807000	-0.461766000
6	1.304929000	1.943361000	-0.249142000	6	1.128265000	1.988811000	-0.426047000
6	0.560505000	0.752772000	-0.021084000	6	-0.017029000	1.025034000	-0.525450000
6	1.243543000	-0.445936000	0.164788000	6	-0.131036000	0.200800000	-1.672562000
8	0.550789000	-1.579202000	0.435586000	6	-1.237380000	-0.581836000	-1.872910000
6	-0.917728000	0.932560000	0.033618000	6	-2.281927000	-0.606413000	-0.913016000
8	-1.606121000	-0.229853000	-0.131195000	6	-2.169602000	0.188574000	0.271656000
6	-3.001397000	-0.231239000	-0.078412000	6	-1.0176514000	1.017454000	0.428355000
8	-1.450510000	2.007079000	0.171134000	6	-3.437880000	-1.410668000	-1.086148000
6	-3.693820000	0.232900000	1.035416000	6	-4.431890000	-1.442003000	-0.137878000

6	-5.082070000	0.122067000	1.058940000	6	-4.311991000	-0.671607000	1.039913000
6	-5.766737000	-0.449912000	-0.013118000	6	-3.205320000	0.119997000	1.239869000
6	-5.055879000	-0.915321000	-1.117695000	8	1.008312000	3.179317000	-0.417496000
6	-3.666919000	-0.807143000	-1.154165000	8	-0.829863000	1.781323000	1.541372000
1	5.336352000	-2.619906000	0.268987000	1	3.690057000	-3.356592000	1.201644000
1	6.578533000	-0.495994000	-0.112996000	1	2.337302000	-1.874978000	2.661817000
1	5.341606000	1.621896000	-0.391408000	1	1.709546000	0.399079000	1.891863000
1	2.920261000	-2.636869000	0.379452000	1	3.752812000	-0.280057000	-1.811329000
1	3.212515000	2.864994000	-0.490548000	1	4.410017000	-2.556268000	-1.036548000
1	0.740962000	2.859698000	-0.366010000	1	0.664891000	0.216958000	-2.407425000
1	1.159731000	-2.285163000	0.673446000	1	-1.325085000	-1.191863000	-2.764476000
1	-3.158167000	0.680043000	1.861983000	1	-3.521812000	-2.008466000	-1.987403000
1	-5.629518000	0.485273000	1.921283000	1	-5.307962000	-2.062694000	-0.286698000
1	-6.847074000	-0.532559000	0.013710000	1	-5.092240000	-0.709999000	1.791077000
1	-5.579655000	-1.363917000	-1.954126000	1	-3.136658000	0.682775000	2.165632000
1	-3.093666000	-1.165758000	-2.000328000	1	-1.658398000	1.902247000	2.014999000
Conformer 7							
6	3.625029000	-1.919549000	-0.750637000				
6	4.374337000	-1.323664000	0.287132000				
6	3.889441000	-0.214448000	0.937761000				
6	2.635212000	0.350391000	0.592315000				
6	1.869587000	-0.260685000	-0.449985000				
6	2.405183000	-1.396294000	-1.111335000				
6	2.134358000	1.511232000	1.238600000				
6	0.922251000	2.032543000	0.878277000				
6	0.116235000	1.412576000	-0.112165000				
6	0.596216000	0.300532000	-0.782931000				
6	-1.176191000	2.087904000	-0.448183000				
8	-1.264413000	3.280570000	-0.566794000				
8	-2.305185000	1.332362000	-0.637243000				
6	-2.522657000	0.094682000	-0.048717000				
6	-3.138425000	-0.876050000	-0.834767000				
6	-3.466328000	-2.105003000	-0.270277000				
6	-3.178209000	-2.365928000	1.070136000				
6	-2.571936000	-1.381654000	1.847571000				
6	-2.249729000	-0.141729000	1.296272000				
8	-0.159627000	-0.208348000	-1.791914000				
1	4.014818000	-2.788551000	-1.267570000				
1	5.335442000	-1.741529000	0.563847000				
1	4.465671000	0.251576000	1.729815000				
1	1.866164000	-1.875331000	-1.923219000				
1	2.729418000	1.983368000	2.011741000				
1	0.543554000	2.931754000	1.348462000				
1	-3.352028000	-0.652072000	-1.872302000				
1	-3.949238000	-2.860632000	-0.879724000				
1	-3.434064000	-3.324267000	1.506644000				
1	-2.358725000	-1.568651000	2.893899000				
1	-1.804820000	0.632493000	1.908649000				
1	0.191363000	-1.053975000	-2.087036000				

Table S3. Optimized Cartesian coordinates (in Å) for the conformers of PNO.

Atomic Number	X	Y	Z	Atomic number	X	Y	Z
Conformer cis				Conformer trans			
6	4.872559000	0.548533000	0.913259000	6	0.456534000	-1.928558000	-0.308689000
6	3.654354000	0.828703000	1.528102000	6	1.760137000	-2.014347000	0.112649000
6	2.451745000	0.433695000	0.942182000	6	2.568734000	-0.851650000	0.177891000
6	2.482637000	-0.244207000	-0.275082000	6	2.018446000	0.414049000	-0.208650000
6	3.694065000	-0.531752000	-0.902332000	6	0.656531000	0.469550000	-0.632776000
6	4.885680000	-0.135273000	-0.302951000	6	-0.099766000	-0.687323000	-0.673743000
8	1.341245000	-0.716311000	-0.908077000	1	4.330086000	-1.863655000	0.905345000
6	0.110210000	-0.120243000	-0.649999000	1	-0.177277000	-2.805067000	-0.372196000
6	-0.140606000	1.235393000	-0.942546000	1	2.184104000	-2.970581000	0.396627000
6	-1.395074000	1.756578000	-0.743676000	6	3.919421000	-0.903524000	0.611172000
6	-2.449988000	0.938416000	-0.256343000	6	2.854673000	1.561129000	-0.160037000
6	-2.200273000	-0.442123000	0.022787000	6	4.159329000	1.472675000	0.264993000
6	-0.888932000	-0.951839000	-0.188847000	6	4.698220000	0.227130000	0.658195000
6	-3.758384000	1.443415000	-0.039853000	1	2.481709000	2.533482000	-0.467917000
6	-4.763481000	0.630153000	0.427830000	1	4.779283000	2.361280000	0.293432000
6	-4.508090000	-0.733223000	0.701657000	1	5.727779000	0.167774000	0.991847000
6	-3.253498000	-1.260745000	0.502916000	1	0.616144000	2.380480000	-0.819879000
8	-0.651317000	-2.266688000	0.069280000	8	0.051357000	1.627560000	-1.017676000
1	5.801915000	0.859039000	1.375725000	8	-1.390899000	-0.655918000	-1.163672000
1	3.632277000	1.355438000	2.475533000	6	-2.430046000	-0.250105000	-0.349721000
1	1.506315000	0.647803000	1.424337000	6	-3.669382000	-0.108696000	-0.976011000
1	3.684567000	-1.060146000	-1.848047000	6	-2.296846000	-0.016788000	1.017763000
1	5.827381000	-0.358399000	-0.791638000	6	-4.778019000	0.268278000	-0.226882000
1	0.668885000	1.847762000	-1.321821000	1	-3.741798000	-0.295018000	-2.040640000
1	-1.594279000	2.798629000	-0.966394000	6	-3.418796000	0.362325000	1.755974000
1	-3.953165000	2.489557000	-0.251800000	1	-1.334863000	-0.130400000	1.501118000
1	-5.757531000	1.032609000	0.587368000	6	-4.660799000	0.506869000	1.143821000
1	-5.308388000	-1.365302000	1.069589000	1	-5.738816000	0.377916000	-0.717499000
1	-3.051240000	-2.303930000	0.709365000	1	-3.313485000	0.543128000	2.820097000
1	0.266299000	-2.451956000	-0.174466000	1	-5.526765000	0.801439000	1.724753000

Table S4. B3LYP/6-311++G(d,p) calculated infrared spectrum of PNO (cis conformer), with approximate normal modes' description.^a

ν^b	I^{IR}	Approximate description ^c
3686	120.4	vOH
3133	6.7	vCH ring3
3130	1.1	vCH ring1
3126	9.1	vCH ring1
3123	5.2	vCH ring2
3118	19.1	vCH ring1
3115	22.6	vCH ring3
3105	9.0	vCH ring1
3104	12.6	vCH rings2-3
3101	5.4	vCH rings2-3
3098	1.7	vCH ring1
3090	0.5	vCH ring3
1635	18.5	v rings2-3, δ CH rings2-3, δ OH
1606	19.0	v rings1-2-3, δ CH rings1-2-3, δ OH
1598	119.1	v rings1-2-3, δ CH rings1-2-3, δ OH
1594	16.5	v ring1, δ CH ring1
1578	27.4	v rings2-3, δ CH rings2-3
1512	16.2	v rings2-3, δ CH rings2-3
1485	122.7	v ring1, δ CH ring1
1464	90.8	v rings2-3, δ CH rings2-3
1454	1.1	v ring1, δ CH ring1
1444	7.0	v rings2-3, δ CH rings2-3, δ OH
1399	59.9	v rings2-3, δ CH rings2-3, δ OH
1380	71.4	v rings2-3, δ CH rings2-3, δ OH
1355	3.5	v rings2-3, δ CH rings2-3, δ OH
1321	12.9	v ring1, δ CH ring1
1298	3.1	v ring1, δ CH ring1
1264	49.5	δ rings2-3, δ CH rings2-3, δ OH
1250	112.2	δ rings2-3, δ CH rings2-3, δ OH, vC-O
1238	176.0	δ rings2-3, δ CH rings2-3, δ OH, vC-O-C asym.
1204	96.7	δ rings1-2-3, δ CH rings1-2-3, δ OH, vC-O
1194	226.0	δ rings1-2-3, δ CH rings1-2-3, δ OH, vC-O
1180	0.4	δ rings1-2-3, δ CH rings1-2-3, vC-O(H), vC-O-C asym.
1159	37.1	δ ring1, δ CH ring1
1153	5.6	δ CH ring1
1147	22.7	δ CH rings2-3, δ OH
1140	2.4	δ CH rings2-3
1076	24.4	δ rings1-2-3, δ CH rings1-2-3
1074	18.2	δ CH ring1
1021	2.6	δ rings1-3, δ CH rings1-3
1019	13.1	δ rings1-3, δ CH rings1-3
993	0.3	δ ring1
974	0.1	γ CH ring3
972	0.4	γ CH ring3
956	1.1	γ CH ring1
953	1.4	γ CH rings2-3
949	95.4	δ rings2-3, δ CH rings2-3, vC-O
934	0.1	γ CH rings2-3
892	4.0	γ CH ring1
865	6.8	δ rings2-3, δ CH rings2-3
856	2.1	γ CH ring1
819	2.8	γ CH ring1
814	38.0	τ rings1-2-3, γ CH rings1-2-3
795	26.9	τ rings2-3, γ CH rings2-3
776	5.5	τ rings2-3, γ CH rings2-3
757	53.4	τ ring1, γ CH ring1, γ CH ring3
742	28.1	γ CH rings1-2-3
720	10.1	δ rings2-3, γ CH ring1
710	7.8	δ rings2-3
689	25.4	τ ring1, γ CH ring1
669	13.0	τ rings2-3, γ CH rings2-3
615	1.9	δ rings1-2-3
612	2.0	δ rings1-2-3, δ C-O-C
577	7.3	δ rings2-3, δ C-O-C

566	8.2	τ rings2-3
531	7.0	δ rings1-2-3, δ C-O(H)
513	2.2	δ rings1-2-3
503	22.2	τ ring1, γ CH ring1, τ OH
494	54.4	τ OH
477	4.0	δ rings1-2-3, δ C-O-C
465	2.5	δ rings2-3
419	10.5	τ rings2-3
412	0.4	τ ring1
336	10.0	ν H $\cdots$ O
319	0.8	γ C-O(H)
271	5.1	δ C-O(H)
252	2.3	Skeletal deformation
231	3.7	rings2-3 sym.butterfly
192	0.5	γ C-O(ph)
149	0.1	rings2-3 asym.butterfly
122	1.3	rings2-3 sym.butterfly
52	0.2	γ C-O(ph), δ C-O-C
37	0.1	τ O-C
17	0.7	τ C-O

^a Frequencies in cm^{-1} ; calculated intensities in km mol^{-1} ; n.obs., not observed; n.i., not investigated. ^b Calculated frequencies were scaled by 0.978. ^c ν , stretching; δ , bending; γ , rocking; τ , torsion; sym., symmetric; asym., anti-symmetric; ph, phenyl ether group. Rings 1, 2 and 3 correspond to the phenyl ether, phenol and benzo aromatic moieties, respectively.