	Definition ^a	Symmetry ^b	Approximate description
\mathbf{S}_1	$v(C_1-C_3)$	А	v(C-C)
S_2	$v(C_1=O_2)+v(C_3=O_4)$	А	v(C=O) s
S_3	$v(C_1=O_2)-v(C_3=O_4)$	В	v(C=O) as
S_4	$v(C_1-C_5)+v(C_3-C_{13})$	А	$v(C-C_{\alpha})$ s
S_5	$v(C_1-C_5)-v(C_3-C_{13})$	В	$v(C-C_{\alpha})$ as
S_6	$\nu(C_7-C_8)+\nu(C_8-O_9)+\nu(O_9-C_5)+\nu(C_5-C_6)+\nu(C_6-C_7)+$	А	v(ring 1) s
	$+\nu(C_{15}-C_{16})+\nu(C_{16}-O_{17})+\nu(O_{17}-C_{13})+\nu(C_{13}-C_{14})+\nu(C_{14}-C_{15})$		
S_7	$\nu(C_7-C_8)+\nu(C_8-O_9)+\nu(O_9-C_5)+\nu(C_5-C_6)+\nu(C_6-C_7)-$	В	v(ring 1) as
	$-\nu(C_{15}-C_{16})-\nu(C_{16}-O_{17})-\nu(O_{17}-C_{13})-\nu(C_{13}-C_{14})-\nu(C_{14}-C_{15})$		
S_8	$\nu(C_7-C_8)+\nu(C_5-C_6)+\nu(C_{15}-C_{16})+\nu(C_{13}-C_{14})$	А	v(ring 2) s
S ₉	$v(C_7-C_8)+v(C_5-C_6)-v(C_{15}-C_{16})-v(C_{13}-C_{14})$	В	v(ring 2) as
S_{10}	$v(C_7-C_8)-v(C_5-C_6)+v(C_{15}-C_{16})-v(C_{13}-C_{14})$	А	v(ring 3) s
S ₁₁	$\nu(C_7-C_8)-\nu(C_5-C_6)-\nu(C_{15}-C_{16})+\nu(C_{13}-C_{14})$	В	v(ring 3) as
S ₁₂	$2\nu(C_6-C_7)-\nu(C_8-O_9)-\nu(O_9-C_5)+2\nu(C_{14}-C_{15})-\nu(C_{16}-O_{17})-\nu(O_{17}-C_{13})$	А	v(ring 4) s
S ₁₃	$2\nu(C_6-C_7)-\nu(C_8-O_9)-\nu(O_9-C_5)-2\nu(C_{14}-C_{15})+\nu(C_{16}-O_{17})+\nu(O_{17}-C_{13})$	В	v(ring 4) as
S ₁₄	$v(C_8-O_9)-v(O_9-C_5)+v(C_{16}-O_{17})-v(O_{17}-C_{13})$	А	v(ring 5) s
S ₁₅	$v(C_8-O_9)-v(O_9-C_5)-v(C_{16}-O_{17})+v(O_{17}-C_{13})$	В	v(ring 5) as
S ₁₆	$\nu(C_6-H_{10})+\nu(C_7-H_{11})+\nu(C_8-H_{12})+\nu(C_{14}-H_{18})+\nu(C_{15}-H_{19})+\nu(C_{16}-H_{20})$	А	v(C-H 1) s
S ₁₇	$\nu(C_6-H_{10})+\nu(C_7-H_{11})+\nu(C_8-H_{12})-\nu(C_{14}-H_{18})-\nu(C_{15}-H_{19})-\nu(C_{16}-H_{20})$	В	v(C-H 1) as
S_{18}	$\nu(C_6-H_{10})-\nu(C_8-H_{12})+\nu(C_{14}-H_{18})-\nu(C_{16}-H_{20})$	А	v(C-H 2) s
S ₁₉	$\nu(C_6-H_{10})-\nu(C_8-H_{12})-\nu(C_{14}-H_{18})+\nu(C_{16}-H_{20})$	В	v(C-H 2) as
S ₂₀	$\nu(C_6-H_{10})-2\nu(C_7-H_{11})+\nu(C_8-H_{12})+\nu(C_{14}-H_{18})-2\nu(C_{15}-H_{19})+\nu(C_{16}-H_{20})$	А	v(C-H 3) s
S ₂₁	$\nu(C_6-H_{10})-2\nu(C_7-H_{11})+\nu(C_8-H_{12})-\nu(C_{14}-H_{18})+2\nu(C_{15}-H_{19})-\nu(C_{16}-H_{20})$	В	v(C-H 3) as
S ₂₂	$\delta(C_5 - C_1 = O_2) - \delta(C_3 - C_1 = O_2) + \delta(C_{13} - C_3 = O_4) - \delta(C_1 - C_3 - C_4)$	А	δ(C=O) s
S ₂₃	$\delta(C_5 - C_1 = O_2) - \delta(C_3 - C_1 = O_2) - \delta(C_{13} - C_3 = O_4) + \delta(C_1 - C_3 - C_4)$	В	δ(C=O) as
S ₂₄	$2\delta(C_5-C_1-C_3)-\delta(C_5-C_1-C_2)-\delta(C_3-C_1-C_2)+2\delta(C_{13}-C_3-C_1)-\delta(C_{13}-C_3-C_4)-\delta(C_1-C_4)-\delta(C_1-C_4)-\delta(C_4)-\delta(C_4)-\delta(C_4)-\delta(C_4)-\delta(C_4)-\delta(C_4$	А	$\delta(CCC_{\alpha})$ s
S ₂₅	$2\delta(C_5-C_1-C_3)-\delta(C_5-C_1-C_2)-\delta(C_3-C_1-C_2)-2\delta(C_{13}-C_3-C_1)+\delta(C_{13}-C_3-C_4)+\delta(C_1-C_3-C_4)$	В	$\delta(CCC_{\alpha})$ as
S ₂₆	$\delta(C_6\text{-}C_5\text{-}C_1)\text{-}\delta(O_9\text{-}C_5\text{-}C_1)\text{+}\delta(C_{14}\text{-}C_{13}\text{-}C_3)\text{-}\delta(O_{17}\text{-}C_{13}\text{-}C_3)$	А	ω(ring) s
S ₂₇	$\delta(C_6\text{-}C_5\text{-}C_1)\text{-}\delta(O_9\text{-}C_5\text{-}C_1)\text{-}\delta(C_{14}\text{-}C_{13}\text{-}C_3)\text{+}\delta(O_{17}\text{-}C_{13}\text{-}C_3)$	В	ω(ring) as
S ₂₈	$\delta(C_8\text{-}O_9\text{-}C_5)\text{-}0.809\delta(C_7\text{-}C_8\text{-}O_9)\text{-}0.809\delta(O_9\text{-}C_5\text{-}C_6)\text{+}0.309\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_6\text{-}C_7)\text{+}0.300\delta(C_7)+$	А	δ(ring 1) s
	$+0.309\delta(C_{5}\text{-}C_{6}\text{-}C_{7})+\delta(C_{16}\text{-}O_{17}\text{-}C_{13})-0.809\delta(C_{15}\text{-}C_{16}\text{-}O_{17})-0.809\delta(O_{17}\text{-}C_{13}\text{-}C_{14})+$		
	$+0.309\delta(C_{14}-C_{15}-C_{16})+0.309\delta(C_{13}-C_{14}-C_{15})$		
S ₂₉	$\delta(C_8\text{-}O_9\text{-}C_5)\text{-}0.809\delta(C_7\text{-}C_8\text{-}O_9)\text{-}0.809\delta(O_9\text{-}C_5\text{-}C_6)\text{+}0.309\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_7\text{-}C_8)\text{+}0.300\delta(C_8\text{-}C_8)\text{+}0.300\delta(C_8)\text{+}0.300\delta$	В	δ(ring 1) as
	$+0.309\delta(C_{5}\text{-}C_{6}\text{-}C_{7})\text{-}\delta(C_{16}\text{-}O_{17}\text{-}C_{13})+0.809\delta(C_{15}\text{-}C_{16}\text{-}O_{17})+0.809\delta(O_{17}\text{-}C_{13}\text{-}C_{14})\text{-}$		
	$-0.309\delta(C_{14}\text{-}C_{15}\text{-}C_{16})\text{-}0.309\delta(C_{13}\text{-}C_{14}\text{-}C_{15})$		
S ₃₀	$-1.118\delta(C_7-C_8-O_9)+1.118\delta(O_9-C_5-C_6)+1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.809\delta(C_5-C_6-C_7)-1.800\delta(C_5-C_7)-1.800\delta(C_5-C_7)-1.800\delta(C_5-C_7)-1.800\delta(C_5-C_7)-1.800\delta(C_5-C_7)-1.800\delta(C_7-C_7)-1.8$	А	δ(ring 2) s
	$-1.118\delta(C_{15}\text{-}C_{16}\text{-}O_{17})+1.118\delta(O_{17}\text{-}C_{13}\text{-}C_{14})+1.809\delta(C_{14}\text{-}C_{15}\text{-}C_{16})-1.809\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14})+1.808\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13}\text{-}C_{15})+1.80\delta(C_{13})+1.$		
S ₃₁	-1.1188(C7-C8-O9)+1.1188(O9-C5-C6)+1.8098(C6-C7-C8)-1.8098(C5-C6-C7)+	В	δ(ring 2) as

Table S1 – Definition of internal symmetry coordinates used in the normal mode analysis of conformers I and III of α -furil.

	$+1.118\delta(C_{15}\text{-}C_{16}\text{-}O_{17})\text{-}1.118\delta(O_{17}\text{-}C_{13}\text{-}C_{14})\text{-}1.809\delta(C_{14}\text{-}C_{15}\text{-}C_{16})\text{+}1.809\delta(C_{13}\text{-}C_{14}\text{-}C_{15})$		
S ₃₂	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{+}\delta(C_6\text{-}C_7\text{-}H_{11})\text{-}\delta(C_8\text{-}C_7\text{-}H_{11})\text{+}\delta(C_7\text{-}C_8\text{-}H_{12})\text{-}$	А	δ(C-H 1) s
	$-\delta(O_9-C_8-H_{12})+\delta(C_{13}-C_{14}-H_{18})-\delta(C_{15}-C_{14}-H_{18})+\delta(C_{14}-C_{15}-H_{19})-\delta(C_{16}-C_{15}-H_{19})+\delta(C_{16}-C_{16}-C_{15}-H_{19})+\delta(C_{16}-C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{16})+\delta(C_{16}-C_{16}-C_{1$		
	$+\delta(C_{15}-C_{16}-H_{20})-\delta(O_{17}-C_{16}-H_{20})$		
S ₃₃	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{+}\delta(C_6\text{-}C_7\text{-}H_{11})\text{-}\delta(C_8\text{-}C_7\text{-}H_{11})\text{+}\delta(C_7\text{-}C_8\text{-}H_{12})\text{-}$	В	δ(C-H 1) as
	$-\delta(O_9-C_8-H_{12})-\delta(C_{13}-C_{14}-H_{18})+\delta(C_{15}-C_{14}-H_{18})-\delta(C_{14}-C_{15}-H_{19})+\delta(C_{16}-C_{15}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-C_{16}-H_{19})-\delta(C_{16}-$		
	$-\delta(C_{15}-C_{16}-H_{20})+\delta(O_{17}-C_{16}-H_{20})$		
S ₃₄	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_8\text{-}H_{12})\text{+}\delta(O_9\text{-}C_8\text{-}H_{12})\text{+}$	А	δ(C-H 2) s
	$+\delta(C_{13}\text{-}C_{14}\text{-}H_{18})\text{-}\delta(C_{15}\text{-}C_{14}\text{-}H_{18})\text{-}\delta(C_{15}\text{-}C_{16}\text{-}H_{20})+\delta(O_{17}\text{-}C_{16}\text{-}H_{20})$		
S ₃₅	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_8\text{-}H_{12})\text{+}\delta(O_9\text{-}C_8\text{-}H_{12})\text{-}$	В	δ(C-H 2) as
	$-\delta(C_{13}-C_{14}-H_{18})+\delta(C_{15}-C_{14}-H_{18})+\delta(C_{15}-C_{16}-H_{20})-\delta(O_{17}-C_{16}-H_{20})$		
S ₃₆	$\delta(C_5 - C_6 - H_{10}) - \delta(C_7 - C_6 - H_{10}) - 2\delta(C_6 - C_7 - H_{11}) + 2\delta(C_8 - C_7 - H_{11}) + \delta(C_7 - C_8 - H_{12}) - \delta(C_7 - C_8 - H_{10}) - \delta(C_8 - H_{10}$	А	δ(C-H 3) s
	$-\delta(O_9-C_8-H_{12})+\delta(C_{13}-C_{14}-H_{18})-\delta(C_{15}-C_{14}-H_{18})-2\delta(C_{14}-C_{15}-H_{19})+2\delta(C_{16}-C_{15}-H_{19})+2\delta$		
	$+\delta(C_{15}-C_{16}-H_{20})-\delta(O_{17}-C_{16}-H_{20})$		
S ₃₇	$\delta(C_5 - C_6 - H_{10}) - \delta(C_7 - C_6 - H_{10}) - 2\delta(C_6 - C_7 - H_{11}) + 2\delta(C_8 - C_7 - H_{11}) + \delta(C_7 - C_8 - H_{12}) - \delta(C_7 - C_8 - H_{10}) - \delta(C_8 - H_{10}$	В	δ(C-H 3) as
	$-\delta(O_9-C_8-H_{12})-\delta(C_{13}-C_{14}-H_{18})+\delta(C_{15}-C_{14}-H_{18})+2\delta(C_{14}-C_{15}-H_{19})-2\delta(C_{16}-C_{15}-H_{19})-2\delta$		
	$-\delta(C_{15}-C_{16}-H_{20})+\delta(O_{17}-C_{16}-H_{20})$		
S ₃₈	$\tau(C_8-C_7-C_6-C_5)-0.809\tau(O_9-C_8-C_7-C_6)-0.809\tau(C_7-C_6-C_5-O_9)+0.309\tau(C_5-O_9-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_7-C_8-C_7)+0.800\tau(C_8-C_8-C_8-C_7)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8-C_8)+0.800\tau(C_8-C_8)+0.800\tau(C_8-C_8)+0.800\tau(C_8-C_8)+0.800\tau(C_8-C_$	А	$\tau(ring \ 1) \ s$
	$+0.309\tau(C_6\text{-}C_5\text{-}O_9\text{-}C_8)+\tau(C_{16}\text{-}C_{15}\text{-}C_{14}\text{-}C_{13})-0.809\tau(O_{17}\text{-}C_{16}\text{-}C_{15}\text{-}C_{14})-$		
	$-0.809\tau(C_{15}\text{-}C_{14}\text{-}C_{13}\text{-}O_{17})+0.309\tau(C_{13}\text{-}O_{17}\text{-}C_{16}\text{-}C_{15})+0.309\tau(C_{14}\text{-}C_{13}\text{-}O_{17}\text{-}C_{16})$		
S ₃₉	$\tau(C_8-C_7-C_6-C_5)-0.809\tau(O_9-C_8-C_7-C_6)-0.809\tau(C_7-C_6-C_5-O_9)+0.309\tau(C_5-O_9-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_5-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.809\tau(C_7-C_8-C_7)+0.807\tau(C_7-C_8-C_7)+0.807\tau(C_7-C_8-C_7)+0.807\tau(C_7-C_8-C_7)+0.807\tau(C_8-C_8-C_7)+0.807\tau(C_8-C_8-C_8)+0.807\tau(C_8-C_8)+0$	В	τ (ring 1) as
	$+0.309\tau(C_6\text{-}C_5\text{-}O_9\text{-}C_8)\text{-}\tau(C_{16}\text{-}C_{15}\text{-}C_{14}\text{-}C_{13})+0.809\tau(O_{17}\text{-}C_{16}\text{-}C_{15}\text{-}C_{14})+$		
	$+0.809\tau(C_{15}\text{-}C_{14}\text{-}C_{13}\text{-}O_{17}\text{)}-0.309\tau(C_{13}\text{-}O_{17}\text{-}C_{16}\text{-}C_{15})-0.309\tau(C_{14}\text{-}C_{13}\text{-}O_{17}\text{-}C_{16})$		
S ₄₀	$1.118\tau(O_9-C_8-C_7-C_6)-1.118\tau(C_7-C_6-C_5-O_9)-1.809\tau(C_5-O_9-C_8-C_7)+$	А	$\tau(ring 2) s$
	$+1.809\tau(C_6-C_5-O_9-C_8)+1.118\tau(O_{17}-C_{16}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14}-C_{15}-C_{14}-C_{15}-C_{14}-C_{15}-C_{14}-C_{15}-C_{14}-C_{15}-C_{14}-C_{15}-C_{15}-C_{14}-C_{15}-C_{15}-C_{14}-C_{15}-C$		
	$-1.809\tau(C_{13}\text{-}O_{17}\text{-}C_{16}\text{-}C_{15})+1.809\tau(C_{14}\text{-}C_{13}\text{-}O_{17}\text{-}C_{16})$		
S_{41}	$1.118\tau(O_9-C_8-C_7-C_6)-1.118\tau(C_7-C_6-C_5-O_9)-1.809\tau(C_5-O_9-C_8-C_7)+$	В	$\tau(ring 2)$ as
	$+1.809\tau(C_6-C_5-O_9-C_8)-1.118\tau(O_{17}-C_{16}-C_{15}-C_{14})+1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})+$		
	+1.809 τ (C ₁₃ -O ₁₇ -C ₁₆ -C ₁₅)-1.809 τ (C ₁₄ -C ₁₃ -O ₁₇ -C ₁₆)		
S ₄₂	$\gamma(C_1-C_6-C_5-O_9)+\gamma(C_3-C_{14}-C_{13}-O_{17})$	А	γ(ring) s
S ₄₃	$\gamma(C_1-C_6-C_5-O_9)-\gamma(C_3-C_{14}-C_{13}-O_{17})$	В	γ(ring) as
S ₄₄	$\tau(O_2=C_1-C_3=O_4)+\tau(O_2=C_1-C_3-C_{13})+\tau(C_5-C_1-C_3-C_{13})+\tau(C_5-C_1-C_3=O_4)$	А	τ(C-C)
S_{45}	$\tau(O_9\text{-}C_5\text{-}C_1\text{-}C_3) + \tau(C_6\text{-}C_5\text{-}C_1\text{-}C_3) + \tau(O_{17}\text{-}C_{13}\text{-}C_3\text{-}C_1) + \tau(C_{14}\text{-}C_{13}\text{-}C_3\text{-}C_1) + \tau(C_{14}\text{-}C_{13}\text{-}C_3) + \tau(C_{14}\text{-}C_{13}\text{-}$	А	$\tau(C-C_{\alpha})$ s
	$+\tau(O_{9}-C_{5}-C_{1}=O_{2})+\tau(C_{6}-C_{5}-C_{1}=O_{2})+\tau(O_{17}-C_{13}-C_{3}=O_{4})+\tau(C_{14}-C_{13}-C_{3}=O_{4})$		
S ₄₆	$\tau(O_9\text{-}C_5\text{-}C_1\text{-}C_3) + \tau(C_6\text{-}C_5\text{-}C_1\text{-}C_3) \text{-}\tau(O_{17}\text{-}C_{13}\text{-}C_3\text{-}C_1) \text{-}\tau(C_{14}\text{-}C_{13}\text{-}C_3\text{-}C_1) +$	В	$\tau(C-C_{\alpha})$ as
	$+\tau(O_9-C_5-C_1=O_2)+\tau(C_6-C_5-C_1=O_2)-\tau(O_{17}-C_{13}-C_3=O_4)-\tau(C_{14}-C_{13}-C_3=O_4)$		
S ₄₇	$\gamma(O_2=C_3-C_1-C_5)+\gamma(O_4=C_1-C_3-C_{13})$	А	γ(C=O) s
S_{48}	$\gamma(O_2=C_3-C_1-C_5)-\gamma(O_4=C_1-C_3-C_{13})$	В	γ(C=O) as
S ₄₉	$\gamma(H_{10}-C_5-C_6-C_7)+\gamma(H_{11}-C_6-C_7-C_8)+\gamma(H_{12}-C_7-C_8-O_9)+$	А	γ(C-H 1) s
	$+\gamma(H_{19}-C_{13}-C_{14}-C_{15})+\gamma(H_{19}-C_{14}-C_{15}-C_{16})+\gamma(H_{20}-C_{15}-C_{16}-O_{17})$		
S ₅₀	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7)+\gamma(H_{11}\text{-}C_6\text{-}C_7\text{-}C_8)+\gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)\text{-}$	В	γ(C-H 1) as
	$-\gamma(H_{19}-C_{13}-C_{14}-C_{15})-\gamma(H_{19}-C_{14}-C_{15}-C_{16})-\gamma(H_{20}-C_{15}-C_{16}-O_{17})$		

\mathbf{S}_{51}	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7)\text{-}\gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)\text{+}\gamma(H_{19}\text{-}C_{13}\text{-}C_{14}\text{-}C_{15})\text{-}\gamma(H_{20}\text{-}C_{15}\text{-}C_{16}\text{-}O_{17})$	А	γ(C-H 2) s
S ₅₂	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7)\text{-}\gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)\text{-}\gamma(H_{19}\text{-}C_{13}\text{-}C_{14}\text{-}C_{15})\text{+}\gamma(H_{20}\text{-}C_{15}\text{-}C_{16}\text{-}O_{17})$	В	γ (C-H 2) as
S ₅₃	$\gamma(H_{10}-C_5-C_6-C_7)-2\gamma(H_{11}-C_6-C_7-C_8)+\gamma(H_{12}-C_7-C_8-O_9)+$	А	γ(C-H 3) s
	$+\gamma(H_{19}-C_{13}-C_{14}-C_{15})-2\gamma(H_{19}-C_{14}-C_{15}-C_{16})+\gamma(H_{20}-C_{15}-C_{16}-O_{17})$		
S ₅₄	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7)\text{-}2\gamma(H_{11}\text{-}C_6\text{-}C_7\text{-}C_8)+\gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)\text{-}$	В	γ (C-H 3) as
	$-\gamma(H_{19}-C_{13}-C_{14}-C_{15})+2\gamma(H_{19}-C_{14}-C_{15}-C_{16})-\gamma(H_{20}-C_{15}-C_{16}-O_{17})$		

^a Normalization factors not shown. ν , bond stretching, δ , bending, γ , rocking, ω , wagging, τ , torsion, s, symmetric, as, asymmetric. See Figure 1 for atom numbering. ^b C₂ symmetry point group.

	Definition ^a	Symmetry ^b	Approximate description
S ₁	$v(C_1-C_3)$	А	v(C-C)
S_2	$v(C_1=O_2)$	А	v(C=O)
S_3	$v(C_3=O_4)$	А	v(C=O)'
S_4	$v(C_1-C_5)+v(C_3-C_{13})$	А	$v(C-C_{\alpha})$
S_5	$v(C_1-C_5)-v(C_3-C_{13})$	А	ν(C-C _α)'
S_6	$\nu(C_7-C_8)+\nu(C_8-O_9)+\nu(O_9-C_5)+\nu(C_5-C_6)+\nu(C_6-C_7)$	А	v(ring 1)
S_7	$\nu(C_{15}-C_{16})+\nu(C_{16}-O_{17})+\nu(O_{17}-C_{13})+\nu(C_{13}-C_{14})+\nu(C_{14}-C_{15})$	А	v(ring 1)'
S_8	$v(C_7-C_8)+v(C_5-C_6)$	А	v(ring 2)
S ₉	$v(C_{15}-C_{16})+v(C_{13}-C_{14})$	А	v(ring 2)'
\mathbf{S}_{10}	$v(C_7-C_8)-v(C_5-C_6)$	А	v(ring 3)
S_{11}	$v(C_{15}-C_{16})-v(C_{13}-C_{14})$	А	v(ring 3)'
S_{12}	$2\nu(C_6-C_7)-\nu(C_8-O_9)-\nu(O_9-C_5)$	А	v(ring 4)
S ₁₃	$2v(C_{14}-C_{15})-v(C_{16}-O_{17})-v(O_{17}-C_{13})$	А	v(ring 4)'
S_{14}	$v(C_8-O_9)-v(O_9-C_5)$	А	v(ring 5)
S_{15}	$v(C_{16}-O_{17})-v(O_{17}-C_{13})$	А	v(ring 5)'
S ₁₆	$v(C_6-H_{10})+v(C_7-H_{11})+v(C_8-H_{12})$	А	v(C-H 1)
S ₁₇	$v(C_{14}-H_{18})+v(C_{15}-H_{19})+v(C_{16}-H_{20})$	А	v(C-H 1)'
S ₁₈	$v(C_6-H_{10})-v(C_8-H_{12})$	А	v(C-H 2)
S ₁₉	$v(C_{14}-H_{18})-v(C_{16}-H_{20})$	А	v(C-H 2)'
S ₂₀	$v(C_6-H_{10})-2v(C_7-H_{11})+v(C_8-H_{12})$	А	v(C-H 3)
S ₂₁	$v(C_{14}-H_{18})-2v(C_{15}-H_{19})+v(C_{16}-H_{20})$	А	v(C-H 3)'
S ₂₂	$\delta(C_5 - C_1 = O_2) - \delta(C_3 - C_1 = O_2) + \delta(C_{13} - C_3 = O_4) - \delta(C_1 - C_3 - C_4)$	А	δ(C=O)
S ₂₃	$\delta(C_5 - C_1 = O_2) - \delta(C_3 - C_1 = O_2) - \delta(C_{13} - C_3 = O_4) + \delta(C_1 - C_3 - C_4)$	А	δ(C=O)'
S ₂₄	$2\delta(C_5\text{-}C_1\text{-}C_3)\text{-}\delta(C_5\text{-}C_1\text{-}C_2)\text{-}\delta(C_3\text{-}C_1\text{-}C_2)+2\delta(C_{13}\text{-}C_3\text{-}C_1)\text{-}\delta(C_{13}\text{-}C_3\text{-}C_4)\text{-}\delta(C_1\text{-}C_3\text{-}C_4)$	А	$\delta(CCC_{\alpha})$
S ₂₅	$2\delta(C_{13}\text{-}C_3\text{-}C_1) - \delta(C_{13}\text{-}C_3\text{-}C_4) - \delta(C_1\text{-}C_3\text{-}C_4) - 2\delta(C_{13}\text{-}C_3\text{-}C_1) + \delta(C_{13}\text{-}C_3\text{-}C_4) + \delta(C_1\text{-}C_3\text{-}C_4) - \delta(C_1\text$	А	$\delta(CCC_{\alpha})'$
S ₂₆	$\delta(C_6\text{-}C_5\text{-}C_1)\text{-}\delta(O_9\text{-}C_5\text{-}C_1)\text{+}\delta(C_{14}\text{-}C_{13}\text{-}C_3)\text{-}\delta(O_{17}\text{-}C_{13}\text{-}C_3)$	А	ω(ring)
S ₂₇	$\delta(C_6\text{-}C_5\text{-}C_1)\text{-}\delta(O_9\text{-}C_5\text{-}C_1)\text{-}\delta(C_{14}\text{-}C_{13}\text{-}C_3)\text{+}\delta(O_{17}\text{-}C_{13}\text{-}C_3)$	А	ω(ring)'
S ₂₈	$\delta(C_8\text{-}O_9\text{-}C_5)\text{-}0.809\delta(C_7\text{-}C_8\text{-}O_9)\text{-}0.809\delta(O_9\text{-}C_5\text{-}C_6)\text{+}0.309\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_8\text{-}C_8)\text{+}0.300\delta(C_8)\text{+}0.300\delta$	А	δ(ring 1)
	$+0.309\delta(C_{5}\text{-}C_{6}\text{-}C_{7})+\delta(C_{16}\text{-}O_{17}\text{-}C_{13})-0.809\delta(C_{15}\text{-}C_{16}\text{-}O_{17})-0.809\delta(O_{17}\text{-}C_{13}\text{-}C_{14})+$		
	$+0.309\delta(C_{14}-C_{15}-C_{16})+0.309\delta(C_{13}-C_{14}-C_{15})$		
S ₂₉	$\delta(C_8\text{-}O_9\text{-}C_5)\text{-}0.809\delta(C_7\text{-}C_8\text{-}O_9)\text{-}0.809\delta(O_9\text{-}C_5\text{-}C_6)\text{+}0.309\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_6\text{-}C_7\text{-}C_8)\text{+}0.300\delta(C_8\text{-}C_8)\text{+}0.300\delta(C_8)\text{+}0.300\delta$	А	δ(ring 1)'
	$+0.309\delta(C_{5}\text{-}C_{6}\text{-}C_{7})\text{-}\delta(C_{16}\text{-}O_{17}\text{-}C_{13})+0.809\delta(C_{15}\text{-}C_{16}\text{-}O_{17})+0.809\delta(O_{17}\text{-}C_{13}\text{-}C_{14})\text{-}$		
	$-0.309\delta(C_{14}\text{-}C_{15}\text{-}C_{16})-0.309\delta(C_{13}\text{-}C_{14}\text{-}C_{15})$		
S ₃₀	$-1.118\delta(C_7-C_8-O_9)+1.118\delta(O_9-C_5-C_6)+1.809\delta(C_6-C_7-C_8)-1.809\delta(C_5-C_6-C_7)$	А	δ(ring 2)
\mathbf{S}_{31}	$-1.118\delta(C_{15}\text{-}C_{16}\text{-}O_{17})+1.118\delta(O_{17}\text{-}C_{13}\text{-}C_{14})+1.809\delta(C_{14}\text{-}C_{15}\text{-}C_{16})-1.809\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14}\text{-}C_{15})+1.808\delta(C_{13}\text{-}C_{14})+1.808\delta(C_{14}\text{-}C_{15}\text{-}C_{16})+1.808\delta(C_{13}\text{-}C_{14})+1.808\delta(C_{14}\text{-}C_{15}\text{-}C_{16})+1.808\delta(C_{13}\text{-}C_{14})+1.808\delta(C_{14}\text{-}C_{15}\text{-}C_{16})+1.808\delta(C_{13}\text{-}C_{14})+1.808\delta(C_{14}\text{-}C_{15}\text{-}C_{16})+1.808\delta(C_{13}\text{-}C_{14})+1.808\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14}\text{-}C_{15})+1.80\delta(C_{14})+1.$	А	δ(ring 2)'
S ₃₂	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{+}\delta(C_6\text{-}C_7\text{-}H_{11})\text{-}\delta(C_8\text{-}C_7\text{-}H_{11})\text{+}\delta(C_7\text{-}C_8\text{-}H_{12})\text{-}\delta(O_9\text{-}C_8\text{-}H_{12})$	А	δ(C-H 1)
S ₃₃	$\delta(C_{13}-C_{14}-H_{18})-\delta(C_{15}-C_{14}-H_{18})+\delta(C_{14}-C_{15}-H_{19})-\delta(C_{16}-C_{15}-H_{19})+\delta(C_{15}-C_{16}-H_{20})-\delta(O_{17}-C_{16}-H_{20})$	А	δ(C-H 1)'

Table S2 – Definition of internal coordinates used in the normal mode analysis of conformer II of α -furil.

S ₃₄	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_8\text{-}H_{12})\text{+}\delta(O_9\text{-}C_8\text{-}H_{12})\text{+}$	А	δ(C-H 2)
	$+ \delta(C_{13}\text{-}C_{14}\text{-}H_{18}) \text{-} \delta(C_{15}\text{-}C_{14}\text{-}H_{18}) \text{-} \delta(C_{15}\text{-}C_{16}\text{-}H_{20}) + \delta(O_{17}\text{-}C_{16}\text{-}H_{20})$		
S ₃₅	$\delta(C_5 - C_6 - H_{10}) - \delta(C_7 - C_6 - H_{10}) - \delta(C_7 - C_8 - H_{12}) + \delta(O_9 - C_8 - H_{12}) - \delta(O_9 - H_{12}) - \delta(O_$	А	δ(C-H 2)'
	$-\delta(C_{13}-C_{14}-H_{18})+\delta(C_{15}-C_{14}-H_{18})+\delta(C_{15}-C_{16}-H_{20})-\delta(O_{17}-C_{16}-H_{20})$		
S ₃₆	$\delta(C_5 - C_6 - H_{10}) - \delta(C_7 - C_6 - H_{10}) - 2\delta(C_6 - C_7 - H_{11}) + 2\delta(C_8 - C_7 - H_{11}) + \delta(C_7 - C_8 - H_{12}) - \delta(C_7 - C_8 - H_{10}) - \delta(C_8 - C_7 - H_{11}) - \delta(C_7 - C_8 - H_{10}) - \delta(C_7 - C_8 - H_{10}) - \delta(C_8 - C_7 - H_{11}) - \delta(C_7 - C_8 - H_{10}) - \delta(C_8 - C_7 - H_{10}) - \delta(C_8 - $	А	δ(C-H 3)
	$-\delta(O_9-C_8-H_{12})+\delta(C_{13}-C_{14}-H_{18})-\delta(C_{15}-C_{14}-H_{18})-2\delta(C_{14}-C_{15}-H_{19})+2\delta(C_{16}-C_{15}-H_{19})+2\delta$		
	$+\delta(C_{15}-C_{16}-H_{20})-\delta(O_{17}-C_{16}-H_{20})$		
S ₃₇	$\delta(C_5\text{-}C_6\text{-}H_{10})\text{-}\delta(C_7\text{-}C_6\text{-}H_{10})\text{-}2\delta(C_6\text{-}C_7\text{-}H_{11})\text{+}2\delta(C_8\text{-}C_7\text{-}H_{11})\text{+}\delta(C_7\text{-}C_8\text{-}H_{12})\text{-}$	А	δ(C-H 3)'
	$-\delta(O_9-C_8-H_{12})-\delta(C_{13}-C_{14}-H_{18})+\delta(C_{15}-C_{14}-H_{18})+2\delta(C_{14}-C_{15}-H_{19})-2\delta(C_{16}-C_{15}-H_{19})-2\delta$		
	$-\delta(C_{15}-C_{16}-H_{20})+\delta(O_{17}-C_{16}-H_{20})$		
S ₃₈	$\tau(C_8\text{-}C_7\text{-}C_6\text{-}C_5)\text{-}0.809\tau(O_9\text{-}C_8\text{-}C_7\text{-}C_6)\text{-}0.809\tau(C_7\text{-}C_6\text{-}C_5\text{-}O_9)\text{+}0.309\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}O_8\text{-}C_8)\text{+}0.300\tau(C_5\text{-}O_8\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau($	А	$\tau(ring 1)$
	$+0.309\tau(C_6-C_5-O_9-C_8)+\tau(C_{16}-C_{15}-C_{14}-C_{13})-0.809\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{15}-C_{14})-0.800\tau(O_{17}-C_{16}-C_{16}-C_{16}-C_{16})-0.800\tau(O_{17}-C_{16}-C_{16}-C_{16}-C_{16})-0.800\tau(O_{17}-C_{16}-C$		
	$-0.809\tau(C_{15}-C_{14}-C_{13}-O_{17})+0.309\tau(C_{13}-O_{17}-C_{16}-C_{15})+0.309\tau(C_{14}-C_{13}-O_{17}-C_{16})$		
S ₃₉	$\tau(C_8\text{-}C_7\text{-}C_6\text{-}C_5)\text{-}0.809\tau(O_9\text{-}C_8\text{-}C_7\text{-}C_6)\text{-}0.809\tau(C_7\text{-}C_6\text{-}C_5\text{-}O_9)\text{+}0.309\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}C_8\text{-}C_7)\text{+}0.300\tau(C_5\text{-}O_9\text{-}O_8\text{-}C_8)\text{+}0.300\tau(C_5\text{-}O_8\text{-}O_8)\text{+}0.300\tau(C_5\text{-}O_8)\text{+}0.300\tau(C_8\text{-}O_8)\text{+}0.300\tau(C_8\text{-}O_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8)\text{+}0.300\tau(C_8$	А	τ(ring 1)'
	$+0.309\tau(C_6-C_5-O_9-C_8)-\tau(C_{16}-C_{15}-C_{14}-C_{13})+0.809\tau(O_{17}-C_{16}-C_{15}-C_{14})+$		
	$+0.809\tau(C_{15}\text{-}C_{14}\text{-}C_{13}\text{-}O_{17})-0.309\tau(C_{13}\text{-}O_{17}\text{-}C_{16}\text{-}C_{15})-0.309\tau(C_{14}\text{-}C_{13}\text{-}O_{17}\text{-}C_{16})$		
S ₄₀	$1.118\tau(O_9-C_8-C_7-C_6)-1.118\tau(C_7-C_6-C_5-O_9)-1.809\tau(C_5-O_9-C_8-C_7)+$	А	$\tau(ring 2)$
	$+1.809\tau(C_6-C_5-O_9-C_8)+1.118\tau(O_{17}-C_{16}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})-1.118\tau(C_{15}-C_{14}-C_{13}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{13}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{13}-C_{15})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{13}-C_{15})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{14}-C_{15}-C_{14})-1.118\tau(C_{15}-C_{15}-C_{14}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15}-C_{15})-1.118\tau(C_{15}-C_{15})-1.118\tau(C_{15}-C_{15}-C_{15})-1.118$		
	$-1.809\tau(C_{13}-O_{17}-C_{16}-C_{15})+1.809\tau(C_{14}-C_{13}-O_{17}-C_{16})$		
S_{41}	$1.118\tau(O_9-C_8-C_7-C_6)-1.118\tau(C_7-C_6-C_5-O_9)-1.809\tau(C_5-O_9-C_8-C_7)+$	А	τ(ring 2)'
	$+1.809\tau(C_6-C_5-O_9-C_8)-1.118\tau(O_{17}-C_{16}-C_{15}-C_{14})+1.118\tau(C_{15}-C_{14}-C_{13}-O_{17})+$		
	+1.809 τ (C ₁₃ -O ₁₇ -C ₁₆ -C ₁₅)-1.809 τ (C ₁₄ -C ₁₃ -O ₁₇ -C ₁₆)		
S ₄₂	$\gamma(C_1-C_5-C_5-O_9)$	А	γ(ring)
S_{43}	$\gamma(C_3-C_{14}-C_{13}-O_{17})$	А	γ(ring)'
S ₄₄	$\tau(O_2=C_1-C_3=O_4)+\tau(O_2=C_1-C_3-C_{13})+\tau(C_5-C_1-C_3-C_{13})+\tau(C_5-C_1-C_3=O_4)$	А	τ(C-C)
S ₄₅	$\tau(O_9\text{-}C_5\text{-}C_1\text{-}C_3) + \tau(C_6\text{-}C_5\text{-}C_1\text{-}C_3) + \tau(O_9\text{-}C_5\text{-}C_1\text{=}O_2) + \tau(C_6\text{-}C_5\text{-}C_1\text{=}O_2) + \tau(C_6\text{-}C_5\text{-}C_1\text{-}O_3) + \tau(C_6\text{-}C_5\text{-}O_3) + \tau(C_6\text{-}O_3\text{-}O_3) + \tau(C_6\text{-}O_3) + \tau(C_6\text{-}O$	А	$\tau(C-C_{\alpha})$
	$+\tau(O_9-C_5-C_1=O_2)+\tau(C_6-C_5-C_1=O_2)+\tau(O_{17}-C_{13}-C_3=O_4)+\tau(C_{14}-C_{13}-C_3=O_4)$		
S ₄₆	$\tau(O_9\text{-}C_5\text{-}C_1\text{-}C_3) + \tau(C_6\text{-}C_5\text{-}C_1\text{-}C_3) - \tau(O_{17}\text{-}C_{13}\text{-}C_3\text{-}C_1) - \tau(C_{14}\text{-}C_{13}\text{-}C_3\text{-}C_1) +$	А	$\tau(C-C_{\alpha})'$
	$+\tau(O_9-C_5-C_1=O_2)+\tau(C_6-C_5-C_1=O_2)-\tau(O_{17}-C_{13}-C_3=O_4)-\tau(C_{14}-C_{13}-C_3=O_4)$		
S_{47}	$\gamma(O_2=C_3-C_1-C_5)+\gamma(O_4=C_1-C_3-C_{13})$	А	γ(C=O)
S_{48}	$\gamma(O_2=C_3-C_1-C_5)-\gamma(O_4=C_1-C_3-C_{13})$	А	γ(C=O)'
S ₄₉	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7) + \gamma(H_{11}\text{-}C_6\text{-}C_7\text{-}C_8) + \gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)$	А	γ(C-H 1)
S ₅₀	$\gamma(H_{19}-C_{13}-C_{14}-C_{15})+\gamma(H_{19}-C_{14}-C_{15}-C_{16})+\gamma(H_{20}-C_{15}-C_{16}-O_{17})$	А	γ(C-H 1)'
S_{51}	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7)\text{-}\gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)+\gamma(H_{19}\text{-}C_{13}\text{-}C_{14}\text{-}C_{15})-\gamma(H_{20}\text{-}C_{15}\text{-}C_{16}\text{-}O_{17})$	А	γ(C-H 2)
S ₅₂	$\gamma(H_{10}\text{-}C_5\text{-}C_6\text{-}C_7)\text{-}\gamma(H_{12}\text{-}C_7\text{-}C_8\text{-}O_9)\text{-}\gamma(H_{19}\text{-}C_{13}\text{-}C_{14}\text{-}C_{15})+\gamma(H_{20}\text{-}C_{15}\text{-}C_{16}\text{-}O_{17})$	А	γ(C-H 2)'
S ₅₃	$\gamma(H_{10}-C_5-C_6-C_7)-2\gamma(H_{11}-C_6-C_7-C_8)+\gamma(H_{12}-C_7-C_8-O_9)$	А	γ(C-H 3)
S ₅₄	$\gamma(H_{19}-C_{13}-C_{14}-C_{15})-2\gamma(H_{19}-C_{14}-C_{15}-C_{16})+\gamma(H_{20}-C_{15}-C_{16}-O_{17})$	А	γ(C-H 3)'

 a Normalization factors not shown. v, bond stretching, $\delta,$ bending, $\gamma,$ rocking, $\omega,$ wagging, $\tau,$ torsion. See Figure 1 for atom numbering. ^b C_1 symmetry point group.

Approximate description	Wavenumber ^b	Intensity	PED ^c
v(C-H 1) as	3209.0	6.5	S ₁₇ (69), S ₁₉ (24)
v(C-H 1) s	3209.0	< 0.1	$S_{16}(69), S_{18}(24)$
v(C-H 2) s	3199.9	< 0.1	$S_{16}(27), S_{18}(71)$
v(C-H 2) as	3199.9	0.8	$S_{17}(27), S_{19}(71)$
v(C-H 3) s	3177.3	< 0.1	$S_{20}(93)$
v(C-H 3) as	3177.2	2.3	$S_{21}(93)$
v(C=O) s	1681.7	48.6	$S_2(86)$
v(C=O) as	1675.2	560.2	$S_{3}(96)$
v(ring 3) s	1554.9	2.1	$S_4(10), S_{10}(65), S_{34}(13)$
v(ring 3) as	1550.8	51.3	$S_{11}(67), S_{35}(14)$
v(ring 2) s	1456.9	2.0	$S_8(55), S_{28}(10)$
v(ring 2) as	1448.1	214.2	$S_9(59), S_{29}(10)$
v(ring 4) s	1396.1	3.3	$S_{12}(39), S_{32}(18), S_{34}(14), S_{36}(10)$
v(ring 4) as	1393.2	85.5	$S_{13}(42), S_{33}(15), S_{35}(16), S_{37}(12)$
$v(C-C_{\alpha})$ s	1299.6	3.2	$S_1(13), S_4(24), S_6(11), S_8(14), S_{22}(15)$
$v(C-C_{\alpha})$ as	1248.3	160.4	$S_5(30), S_7(33)$
$\delta(C-H_1)$ s	1219.8	0.3	$S_{32}(67)$
δ (C-H 1) as	1219.2	1.7	S ₃₃ (64)
v(ring 5) s	1164.7	0.1	$S_{14}(57), S_{34}(19)$
v(ring 5) as	1162.3	12.7	$S_9(14), S_{15}(50), S_{35}(20)$
v(ring 1) s	1098.9	< 0.1	$S_{6}(64)$
δ (C-H 2) as	1088.6	48.9	$S_7(30), S_{11}(11), S_{15}(14), S_{35}(15), S_{37}(12)$
δ(C-H 3) s	1063.2	0.1	$S_1(12), S_8(11), S_{14}(10), S_{36}(32)$
$\delta(C-H_3)$ as	1021.2	161.7	$S_{13}(28), S_{35}(16), S_{37}(47)$
$\delta(C-H_2)$ s	1008.8	3.8	$S_{12}(35), S_{34}(24), S_{36}(24)$
v(ring 1) as	928.2	39.3	$S_7(19), S_{13}(11), S_{15}(20), S_{20}(17)$
$\delta(\text{ring 1})$ s	906.7	2.2	$S_{14}(10), S_{28}(41), S_{30}(11)$
γ (C-H 3) as	898.8	14	$S_{52}(14)$, $S_{54}(89)$
$\gamma(C-H_3)$ s	898.0	3.6	$S_{51}(12), S_{53}(93)$
$\delta(\operatorname{ring} 2)$ as	884.3	26.5	$S_{29}(38), S_{31}(51)$
$\delta(\operatorname{ring} 2)$ s	883.2	0.8	$S_{28}(25), S_{30}(64)$
γ (C-H 2) as	853.1	<0.1	$S_{48}(10), S_{52}(67), S_{54}(22)$
$\gamma(C-H_2)$ s	847.2	7.1	$S_{51}(83), S_{53}(18)$
$\gamma(C=O)$ as	809.0	27.1	$S_{48}(58), S_{52}(14)$
γ (C-H 1) s	764.2	121.2	S ₄₉ (86)
γ (C-H 1) as	763.7	3.7	$S_{50}(87)$
$\delta(ring 1)$ as	758.2	243.6	$S_{23}(28), S_{29}(11), S_{31}(13), S_{48}(12)$
v(C-C)	687.8	2.4	$S_{24}(14), S_{40}(25), S_{42}(17), S_{47}(19), S_{1}(10)$
$\tau(ring 2)$ s	634.6	1.5	$S_{24}(24), S_{40}(31)$
$\tau(\operatorname{ring} 2)$ as	617.2	2.8	$S_{39}(12), S_{41}(76)$
$\tau(\text{ring } 1)$ s	590.0	18.9	$S_{38}(87), S_{40}(23)$
$\tau(\text{ring 1})$ as	589.5	0.4	$S_{20}(95), S_{41}(15)$
$\omega(ring)$ as	502.3	4.8	$S_{5}(32), S_{23}(19), S_{27}(13), S_{20}(12)$
$\gamma(C=0)$ s	466.1	14 7	$S_4(12), S_{40}(17), S_{47}(43)$
$\delta(C=0)$ s	375 5	2.5	$S_1(21)$, $S_{22}(55)$
$\omega(ring)$ s	280.6	0.2	$S_1(22), S_{22}(37)$ $S_1(22), S_4(18), S_{26}(37)$
$\delta(C=0)$ as	278.8	21.5	$S_{22}(37)$ $S_{25}(24)$ $S_{27}(34)$
$\delta(CCC_{\mu})$ s	193.0	0.6	$S_{23}(37), S_{23}(27), S_{27}(37)$ $S_{24}(41), S_{26}(38)$
$\gamma(ring)$ as	171.2	0.0	$S_{42}(80)$
$\gamma(ring)$ as	156.8	0.1	$S_{42}(67), S_{47}(19)$
$\delta(CCC_{\star})$ as	126.0	2.5	$S_{25}(45), S_{27}(26), S_{46}(24)$
$\tau(\mathbf{C}-\mathbf{C}_{\alpha})$ as	74.0	1.5	$S_{25}(17), S_{27}(25), S_{40}(27)$
$\tau(C-C_{\alpha})$ as	60.7	0.5	$S_{45}(97)$
τ(C-C)	21.7	6.5	S ₄₄ (91)

Table S3 - Calculated [scaled, DFT(B3LYP)/6-311++G(d,p)] wavenumbers, IR intensities and Potential Energy Distributions (PED) for conformer I of α -furil.^a

^a Wavenumbers in cm⁻¹, calculated intensities in km mol⁻¹, v, bond stretching, δ , bending, γ , rocking, ω ,

wagging, τ , torsion, s, symmetric, as, asymmetric. See Table S1 for definition of internal coordinates and Figure 1 for atom numbering. ^b Scaled (0.978). ^c Only PED values greater than 10 % are given.

$ \begin{array}{cccc} v(C-H 1) & 3203.5 & <0.1 & S_{16}(77), S_{18}(21) \\ v(C+11)' & 3202.9 & 0.2 & S_{17}(44) \\ v(C+12)' & 3195.9 & 1.1 & S_{16}(21), S_{18}(78) \\ v(C-H 2)' & 3197.2 & 1.4 & S_{21}(97) \\ v(C-H 3)' & 3177.2 & 1.4 & S_{21}(97) \\ v(C-O)' & 1692.3 & 265.3 & S_{8}(89) \\ v(C=O)' & 1692.3 & 302.6 & S_{8}(89) \\ v(C=O)' & 1692.3 & 302.6 & S_{8}(89) \\ v(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{51}(12) \\ v(ring 2)' & 1456.9 & 60.2 & S_{62}(25) \\ v(ring 2)' & 1456.9 & 60.2 & S_{62}(25), S_{63}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{16}(40), S_{53}(15), S_{54}(10) \\ v(C-C_u)' & 1298.5 & 21.8 & S_{1}(12), S_{63}(14), S_{54}(10) \\ v(C-C_u)' & 1298.5 & 21.8 & S_{1}(12), S_{64}(14), S_{52}(10) \\ v(C-C_u)' & 1298.5 & 10.1 & S_{62}(25), S_{53}(43) \\ v(ring 5)' & 1163.1 & 4.5 & S_{64}(10), S_{16}(43), S_{54}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{64}(10), S_{16}(43), S_{14}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{64}(10), S_{16}(43), S_{14}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{64}(10), S_{16}(43), S_{14}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{64}(10), S_{16}(3) \\ v(ring 1)' & 1028.4 & 26.5 & S_{7}(28), S_{16}(3), S_{53}(11) \\ v(ring 1)' & 1018.5 & 33.1 & S_{17}(23), S_{63}(21), S_{77}(23) \\ \delta(C+H 2)' & 1008.4 & 26.5 & S_{12}(28), S_{16}(13), S_{54}(14) \\ \delta(ring 1)' & 993.8 & 11.5 & S_{11}(1), S_{16}(14), S_{26}(24) \\ v(ring 1)' & 993.8 & 11.5 & S_{11}(10), S_{26}(16) \\ \delta(ring 1)' & 993.8 & 11.4 & S_{16}(23), S_{16}(53) \\ \delta(ring 2)' & 884.3 & 14.9 & S_{26}(27), S_{36}(24) \\ v(ring 1)' & 773.8 & 22.42 & S_{23}(19), S_{54}(25) \\ \delta(C-H 1)' & 760.8 & 76.7 & S_{64}(82) \\ v(C-C)' & 718.2 & 9.9 & S_{11}(3), S_{16}(15), S_{51}(25) \\ v(C-C)' & 718.2 & 9.9 & S_{11}(3), S_{16}(15), S_{16}(15) \\ v(ring 1)' & 778.3 & 22.42 & S_{23}(19), S_{54}(2) \\ v(C-C)' & 718.2 & 9.9 & S_{16}(3), S_{16}(15) \\ v(C-G)' & 489.5 & 2.8 & S_{64}(23), S_{66}(25) \\ v(C-C)' & 718.2 & 9.2 & S_{16}(3), S_{16}(1), S_{26}(10) \\ v(ring 1)' & 758.3 & 2.42.4 & S_{24}(10), S_{26}(10) \\ v(C-C)' & 489.5 & 2.8 & S_{64}(23), S_{64}(23) \\ v(ring 1)' & 758.3 & 2.42.4 & S_{24}(10), $	Approximate description	Wavenumber ^b	Intensity	PED ^c
$ \begin{array}{cccc} v(C-H 1)' & 3202.9 & 0.2 & S_{1}(0.4) & v(C-H 2)' & 3195.9 & 1.1 & S_{10}(21), S_{10}(7.8) & v(C-H 2)' & 3191.3 & 1.1 & S_{10}(21), S_{10}(7.8) & v(C-H 3)' & 3176.2 & 0.8 & S_{20}(99) & v(C-O)' & 1692.3 & 265.3 & S_{2}(88) & v(C=O)' & 1673.2 & 302.6 & S_{2}(89) & v(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{31}(12) & v(ring 2)' & 1456.9 & 60.2 & S_{10}(29), S_{30}(10) & v(ring 4)' & 1394.5 & 37.1 & S_{10}(40), S_{32}(14), S_{31}(10) & v(ring 4)' & 1394.5 & 37.1 & S_{11}(40), S_{32}(14), S_{31}(10) & v(C-C_{u})' & 1298.5 & 21.8 & S_{1}(12), S_{4}(24), S_{22}(14), S_{31}(10) & v(C-C_{u})' & 1298.5 & 21.8 & S_{1}(12), S_{4}(24), S_{22}(10) & v(C-C_{u})' & 1298.5 & 21.8 & S_{1}(12), S_{4}(24), S_{22}(16) & v(ring 5)' & 1163.1 & 4.5 & S_{6}(10), S_{16}(49), S_{16}(13) & v(ring 5)' & 1163.1 & 4.5 & S_{6}(10), S_{16}(49), S_{16}(13) & v(ring 5)' & 1165.1 & 4.5 & S_{6}(10), S_{16}(49), S_{16}(13) & v(ring 5)' & 1165.5 & 10.1 & S_{12}(25), S_{13}(13) & v(ring 1) & 1105.9 & 24.7 & S_{6}(50), S_{1}(13) & v(ring 5)' & 1165.5 & 10.1 & S_{12}(25), S_{31}(13) & v(ring 1) & 1105.9 & 24.7 & S_{6}(30), S_{10}(13) & v(ring 1)' & 1088.9 & 3.7 & S_{12}(27), S_{36}(21), S_{36}(21) & S_{36}(14) & S_{36}(14) & S_{36}(14) & S_{36}(14) & S_{36}(15) & S_{16}(14), S_{16}(16) & S_{16}(17), S_{16}(16) & S_{16}(16) & S_{16}(16) & S_{16}(17), S_{$	v(C-H 1)	3203.5	<0.1	$S_{16}(77), S_{18}(21)$
$ \begin{array}{cccc} v(C-H 2)' & 3195.9 & 1.1 & S_{19}(94) \\ v(C-H 2)' & 3177.2 & 1.4 & S_{21}(97) \\ v(C-H 3)' & 3177.2 & 1.4 & S_{21}(97) \\ v(C-H 3)' & 3176.2 & 0.8 & S_{20}(99) \\ v(C=O)' & 1692.3 & 265.3 & S_{16}(88) \\ v(C=O)' & 1673.2 & 302.6 & S_{26}(89) \\ v(ring 3)' & 1564.3 & 63.4 & S_{4}(10), S_{10}(55) \\ v(ring 2)' & 1456.9 & 60.2 & S_{6}(29) \\ v(ring 2)' & 1456.9 & 60.2 & S_{6}(29), S_{5}(15) \\ v(ring 2)' & 1456.9 & 60.2 & S_{12}(2), S_{3}(0), S_{34}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{17}(40), S_{27}(10) \\ v(rC-Q_{4})' & 1298.5 & 21.8 & S_{1}(12), S_{17}(15), S_{16}(10) \\ v(ring 4)' & 1298.5 & 21.8 & S_{1}(12), S_{17}(14), S_{22}(15) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{37}(66) \\ \delta(C-H 1)' & 1223.6 & 2.4 & S_{37}(66) \\ \delta(C-H 1)' & 1223.6 & 2.4 & S_{31}(63), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{16}(49), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{16}(49), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{16}(49), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{16}(49), S_{34}(13) \\ v(ring 1) & 105.9 & 4.7 & S_{6}(50), S_{5}(19) \\ \delta(C-H 2)' & 1088.4 & 26.5 & S_{7}(28), S_{15}(13), S_{35}(11) \\ \delta(C-H 3)' & 1088.4 & 26.5 & S_{7}(28), S_{15}(13), S_{35}(11) \\ \delta(C-H 3)' & 1085.8 & 81.1 & S_{12}(28), S_{26}(1), S_{17}(39) \\ \delta(C-H 3)' & 1085.8 & 11.5 & S_{11}(1), S_{16}(10), S_{20}(16) \\ \delta(ring 1) & 905.9 & 11.2 & S_{36}(49) \\ \gamma(ring 1)' & 938.3 & 11.5 & S_{17}(11), S_{15}(10), S_{20}(16) \\ \delta(ring 1)' & 938.3 & 11.5 & S_{17}(11), S_{16}(10), S_{20}(16) \\ \delta(ring 2)' & 884.1 & 4.8 & S_{26}(23), S_{36}(15) \\ \delta(ring 2)' & 884.1 & 4.8 & S_{26}(23), S_{36}(15) \\ \delta(ring 1)' & 738.3 & 24.2 & S_{27}(49) \\ \gamma(C-H 1)' & 760.8 & 76.5 & S_{26}(84) \\ \gamma(C-H 2)' & 849.2 & 7.4 & S_{46}(8), S_{51}(57), S_{51}(12), S_{77}(12) \\ \gamma(C-H 1)' & 780.4 & 4.5 & S_{20}(23), S_{30}(12) \\ \gamma(C-H 1)' & 780.4 & 4.5 & S_{20}(23), S_{30}(12) \\ \gamma(C-H 1)' & 780.4 & 4.5 & S_{26}(23), S_{36}(13), S_{27}(10) \\ \gamma(C-C)' & 411.9 & 51.3 & S_{26}(23), S_{26}(13), S_{26}(10) \\ \gamma(C-H 1)' & 590.4 & 1.47 & S_{39}(83), S_{61}(13), $	$v(C-H 1)^{2}$	3202.9	0.2	S ₁₇ (94)
$ \begin{array}{cccc} v(C-H 2) & 3191.3 & 1.1 & S_{16}(21), S_{18}(78) \\ v(C-H 3)' & 3177.2 & 1.4 & S_{21}(97) \\ v(C-O)' & 1692.3 & 265.3 & S_{0}(89) \\ v(C-O)' & 1673.2 & 302.6 & S_{7}(89) \\ v(ring 3) & 1562.3 & 63.4 & S_{4}(10), S_{10}(55) \\ v(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{51}(12) \\ v(ring 2)' & 1456.9 & 60.2 & S_{62}(22), S_{63}(0), S_{94}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{13}(40), S_{31}(15), S_{34}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{13}(40), S_{31}(15), S_{34}(10) \\ v(rc-C_{\alpha})' & 1248.9 & 116.3 & S_{5}(26), S_{61}(7), S_{7}(14), S_{32}(15) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(66) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(66) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(61) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(61) \\ \delta(C-H 1)' & 1223.6 & 2.4 & S_{64}(3), S_{54}(13) \\ v(ring 5)' & 1165.1 & 4.5 & S_{61}(10, S_{16}(43), S_{33}(15) \\ v(ring 5)' & 1165.5 & 10.1 & S_{62}(3), S_{13}(3), S_{33}(13) \\ v(ring 1) & 1105.9 & 3.7 & S_{12}(23), S_{34}(13) \\ v(ring 5)' & 1155.5 & 10.1 & S_{62}(3), S_{13}(13) \\ v(ring 1)' & 1088.4 & 2.6.5 & S_{7}(28), S_{16}(13), S_{35}(11) \\ \delta(C-H 3)' & 1088.9 & 3.7 & S_{12}(2), S_{36}(27) \\ \delta(C-H 12)' & 1008.9 & 40.5 & S_{12}(27), S_{34}(21), S_{36}(24) \\ v(ring 1)' & 938.3 & 11.5 & S_{11}(1), S_{37}(39) \\ \delta(C-H 3)' & 1085.9 & 3.1 & S_{12}(28), S_{34}(14) \\ v(ring 1)' & 938.3 & 11.5 & S_{11}(1), S_{35}(10) \\ v(ring 1)' & 938.3 & 11.4 & S_{28}(98) \\ \delta(ring 1)' & 905.9 & 13.2 & S_{28}(40) \\ v(C-H 3)' & 888.9 & 1.4 & S_{28}(23), S_{36}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{35}(56) \\ \sigma(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{35}(56) \\ \sigma(ring 1)' & 759.3 & 45.3 & S_{69}(8) \\ \delta(ring 1)' & 759.3 & 45.3 & S_{69}(8) \\ \delta(ring 1)' & 759.3 & 45.3 & S_{69}(8) \\ \delta(ring 1)' & 759.3 & 45.3 & S_{69}(8) \\ \delta(ring 1)' & 759.3 & 45.3 & S_{69}(23), S_{61}(15) \\ v(C-C)' & 718.2 & 9.9 & S_{11}(1), S_{64}(15), S_{61}(12) \\ v(C-C)' & 718.2 & 9.9 & S_{11}(1), S_{64}(12), S_{7}(12) \\ v(C-C)' & 718.2 & 9.9 & S_{11}(1), S_{64}(12), S_{7}(12) \\ v(C-C)' & 718.2 & 9.9 & S_{11}(1), S_{64}(12), S_{7}(12) \\ v(C-C)' & 718$	v(C-H 2)'	3195.9	1.1	$S_{19}(94)$
$ \begin{array}{cccc} v(C-H3) & 3177.2 & 1.4 & S_{21}(97) & M \\ v(C-H3) & 3176.2 & 0.8 & S_{60}(99) \\ v(C=O) & 1692.3 & 265.3 & S_{6}(88) \\ v(ring 3) & 1562.3 & 63.4 & S_{6}(10), S_{10}(55) \\ v(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{34}(12) \\ v(ring 2)' & 1456.9 & 60.2 & S_{6}(22), S_{6}(30), S_{34}(10) \\ v(ring 2)' & 1456.9 & 60.2 & S_{6}(22), S_{6}(30), S_{34}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{13}(40), S_{34}(15), S_{34}(10) \\ v(rcC_{4})' & 1294.5 & 37.1 & S_{13}(40), S_{34}(15), S_{34}(10) \\ v(rcC_{4})' & 1295.8 & 21.8 & S_{12}(22), S_{22}(44), S_{22}(10) \\ v(C-C_{4})' & 1248.9 & 116.3 & S_{12}(26), S_{6}(17), S_{7}(14), S_{32}(15) \\ \delta(C+H1)' & 1223.6 & 2.2 & S_{33}(66) \\ \delta(C+H1)' & 1216.3 & 3.4 & S_{14}(25), S_{34}(3) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{34}(13), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{34}(3), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{34}(3), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{34}(3), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{4}(10), S_{34}(3), S_{34}(13) \\ v(ring 1) & 1005.9 & 24.7 & S_{4}(20), S_{4}(19) \\ \delta(C+H2)' & 1008.9 & 40.5 & S_{12}(27), S_{34}(21), S_{37}(39) \\ \delta(C+H2)' & 1008.9 & 40.5 & S_{12}(27), S_{34}(21), S_{35}(24) \\ v(ring 1)' & 905.9 & 13.2 & S_{24}(40) \\ v(C-H3)' & 804.0 & 1.7 & S_{33}(93) \\ \delta(C+H2)' & 1008.9 & 40.5 & S_{12}(27), S_{34}(21), S_{35}(24) \\ v(ring 1)' & 905.9 & 13.2 & S_{24}(40) \\ v(C-H3)' & 804.1 & 4.8 & S_{23}(23), S_{36}(50) \\ \delta(ring 1)' & 905.9 & 13.2 & S_{24}(40) \\ v(C-H1)' & 810.7 & 6.5 & S_{22}(34) \\ \delta(ring 2)' & 883.1 & 14.9 & S_{34}(23), S_{35}(15) \\ \delta(ring 2)' & 884.1 & 4.8 & S_{34}(23), S_{34}(15) \\ \delta(ring 2)' & 813.3 & 14.9 & S_{34}(23), S_{34}(56), S_{31}(26) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{34}(12), S_{45}(17), S_{45}(17) \\ v(C-H1)'' & 760.8 & 7.7 & S_{6}(82) \\ v(C-H1)'' & 760.8 & 7.7 & S_{6}(82) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{34}(11), S_{44}(13) \\ v(ring 1)' & 589.4 & 2.3 & S_{34}(9), S_{34}(11), S_{45}(13) \\ v(ring 1)' & 589.4 & 2.3 & S_{34}(3), S_{34}(11) \\ \delta(C=O'' & 489.5 $	v(C-H 2)	3191.3	1.1	$S_{16}(21), S_{18}(78)$
$ \begin{array}{cccc} v(C-H3) & 3176.2 & 0.8 & S_{20}(99) \\ v(C=O)' & 1692.3 & 265.3 & S_{5}(88) \\ v(ring 3) & 1562.3 & 63.4 & S_{4}(10), S_{6}(55) \\ v(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{3}(12) \\ v(ring 2)' & 1456.9 & 66.2 & S_{6}(22), S_{6}(30), S_{3}(10) \\ v(ring 2)' & 1456.9 & 66.2 & S_{6}(22), S_{6}(30), S_{3}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{14}(40), S_{12}(14), S_{12}(10) \\ v(rcC_{c_{4}})' & 1298.5 & 21.8 & S_{1}(12), S_{1}(41), S_{12}(10) \\ v(C-C_{c_{4}})' & 1298.5 & 21.8 & S_{1}(2), S_{1}(24), S_{22}(10) \\ v(ring 5)' & 1163.1 & 4.5 & S_{6}(10), S_{14}(4), S_{12}(15) \\ \delta(C-H1)' & 1223.6 & 2.2 & S_{13}(66) \\ \delta(C-H1)' & 1223.6 & 2.2 & S_{14}(63) \\ v(ring 5)' & 1163.1 & 4.5 & S_{6}(10), S_{1}(49), S_{24}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{6}(10), S_{1}(49), S_{24}(13) \\ v(ring 1) & 1105.9 & 24.7 & S_{6}(50), S_{6}(43) \\ v(ring 1) & 1105.9 & 24.7 & S_{6}(50), S_{6}(13) \\ v(ring 1) & 1105.9 & 24.7 & S_{6}(50), S_{6}(13) \\ v(ring 1) & 1058.9 & 3.7 & S_{1}(12), S_{14}(33), S_{25}(11) \\ \delta(C-H3)' & 108.5 & 83.1 & S_{12}(28), S_{24}(11), S_{15}(39) \\ \delta(C-H3)' & 108.5 & 83.1 & S_{12}(28), S_{26}(11), S_{15}(24) \\ v(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{15}(10), S_{20}(16) \\ \delta(ring 1) & 905.9 & 13.2 & S_{26}(40) \\ v(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{15}(10), S_{20}(16) \\ \delta(ring 1) & 905.9 & 13.2 & S_{26}(40) \\ v(C-H3)' & 888.9 & 1.4 & S_{26}(23), S_{30}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{30}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{30}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{31}(26) \\ v(C-H1)' & 760.8 & 76.7 & S_{26}(84) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{20}(12), S_{46}(22) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{26}(21), S_{26}(21) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{26}(21), S_{27}(21) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{26}(21), S_{27}(10) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{26}(21), S_{27}(10) \\ v(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{26}(13), S_{27}(10) \\ v(C-C)' & 489.5 & 2.8 & S_{2}(29), S_{21}(15), S_{26}(31) \\ v(ring)' & 285.5 & 3.1 & S_{1}(13), S_{2$	$v(C-H_3)^{2}$	3177.2	1.4	$S_{21}(97)$
$\begin{array}{cccc} V(C=O) & 1692.3 & 265.3 & S_2(88) \\ V(C=O) & 1673.2 & 302.6 & S_2(89) \\ V(ring 3) & 1562.3 & 63.4 & S_4(10), S_{10}(55) \\ V(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{13}(12) \\ V(ring 2)' & 1456.9 & 60.2 & S_6(22), S_6(30), S_{14}(10) \\ V(ring 2)' & 1456.9 & 60.2 & S_6(22), S_6(30), S_{14}(10) \\ V(ring 4)' & 1394.5 & 37.1 & S_{13}(40), S_{13}(15), S_{14}(10) \\ V(C=C_0) & 1298.5 & 21.8 & S_1(12), S_4(24), S_{22}(10) \\ V(C=C_0)' & 1248.9 & 116.3 & S_6(26), S_6(17), S_7(14), S_{32}(15) \\ \delta(C=H1)' & 1223.6 & 2.2 & S_{13}(66) \\ \delta(C=H1)' & 1223.6 & 2.2 & S_{13}(66) \\ \delta(C=H1)' & 1223.6 & 2.2 & S_{13}(56) \\ V(ring 5)' & 1163.1 & 4.5 & S_6(10), S_{14}(49), S_{34}(13) \\ V(ring 5)' & 1165.5 & 10.1 & S_6(23), S_{16}(13), S_{35}(13) \\ V(ring 1) & 1105.9 & 24.7 & S_6(50), S_7(19) \\ \delta(C=H2)' & 1088.4 & 26.5 & S_{7}(28), S_{13}(13), S_{13}(11) \\ \delta(C=H3)' & 1018.5 & 83.1 & S_{13}(28), S_{13}(11), S_{13}(10) \\ \delta(C=H3)' & 1018.5 & 83.1 & S_{13}(28), S_{13}(11), S_{13}(10) \\ \delta(C=H3)' & 1008.9 & 40.5 & S_{12}(27), S_{36}(27) \\ \delta(C=H2)' & 1008.9 & 40.5 & S_{12}(27), S_{36}(24) \\ V(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{13}(10), S_{20}(16) \\ \delta(ring 1) & 905.9 & 13.2 & S_{24}(9) \\ V(C=H3)' & 888.9 & 1.4 & S_{4}(98) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{13}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{36}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{36}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{36}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{36}(26) \\ V(C-H1)' & 760.8 & 76.7 & S_{36}(82) \\ V(C-H1)' & 760.8 & 76.7 & S_{36}(82) \\ V(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{36}(12), S_{36}(12) \\ V(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{36}(12), S_{37}(12) \\ V(C-C)' & 718.2 & 9.9 & S_{1}(10), S_{36}(12), S_{36}(13) \\ V(ring 1)' & 580.4 & 14.7 & S_{36}(83), S_{36}(13) \\ S(ring 1)' & 758.3 & 22.42 & S_{22}(19), S_{36}(12), S_{37}(10) \\ V(C=O)' & 489.5 & 2.4 & S_{24}(19), S_{36}(13), S_{26}(10) \\ V(C=O)' & 489.5 & 2.4 & S_{2}(30), S_{36}(11) \\ \delta(C=O')' & 489.5 & 2.4 & S_{2}(30), S_{36}(11) \\ \delta(C=O')' & 489.5 & 2.4 $	v(C-H 3)	3176.2	0.8	$S_{20}(99)$
$ \begin{array}{cccc} v(C=0) & 1673.2 & 302.6 & S_2(89) \\ v(ring 3) & 1562.3 & 63.4 & S_4(10), S_{10}(55) \\ v(ring 2)' & 1554.9 & 54.7 & S_{11}(58), S_{35}(12) \\ v(ring 2)' & 1456.9 & 60.2 & S_8(22), S_6(30), S_{34}(10) \\ v(ring 4)' & 1394.5 & 37.1 & S_{12}(40), S_{31}(15), S_{31}(10) \\ v(rc-C_a) & 1288.5 & 21.8 & S_1(12), S_4(24), S_{32}(10) \\ v(C-C_a)' & 1248.9 & 116.3 & S_2(26), S_6(17), S_7(14), S_{32}(15) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(66) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(66) \\ \delta(C-H 1)' & 1223.6 & 2.2 & S_{33}(66) \\ \delta(C-H 1)' & 1223.6 & 2.4 & S_{34}(25), S_{32}(43) \\ v(ring 5)' & 1163.1 & 4.5 & S_6(10), S_{34}(49), S_{34}(13) \\ v(ring 5)' & 1165.1 & 4.5 & S_6(10), S_{34}(49), S_{34}(13) \\ v(ring 5)' & 1165.5 & 10.1 & S_8(23), S_{34}(33), S_{35}(13) \\ v(ring 1) & 1105.9 & 24.7 & S_6(50), S_7(19) \\ \delta(C-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{35}(11), S_{35}(11) \\ \delta(C-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{35}(11), S_{37}(39) \\ \delta(C-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{35}(11), S_{37}(39) \\ \delta(C-H 3)' & 1018.5 & S_{11} & S_{13}(28), S_{36}(16) \\ \delta(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{35}(24) \\ v(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{35}(12), S_{36}(24) \\ v(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{35}(12), S_{36}(24) \\ v(ring 1)' & 938.3 & 11.5 & S_{7}(11), S_{15}(10), S_{26}(16) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{30}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{30}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{26}(23), S_{30}(56) \\ \gamma(C-H 2)' & 840.7 & 6.5 & S_{5}(84) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{5}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(81) \\ \delta(ring 1)' & 738.3 & 224.2 & S_{31}(10), S_{41}(13), S_{42}(17), S_{42}(22) \\ \gamma(ring 1)' & 590.4 & 14.7 & S_{50}(50), S_{61}(1), S_{62}(10) \\ \gamma(C-C)' & 489.5 & 2.8 & S_{62}(2), S_{61}(1$	v(C=O)	1692.3	265.3	$S_3(88)$
	v(C=O)	1673.2	302.6	$S_2(89)$
$\begin{array}{cccc} v(ring 3)' & 1554.9 & 54.7 & S_{11}(58), S_{32}(12) \\ v(ring 2)' & 1456.9 & 60.2 & S_{8}(22), S_{8}(30), S_{34}(10) \\ v(ring 2)' & 1450.2 & 181.6 & S_{8}(27), S_{8}(29) \\ v(ring 4)' & 1394.5 & 37.1 & S_{13}(40), S_{33}(15), S_{34}(10) \\ v(rc.C_a)' & 1298.5 & 21.8 & S_{1}(12), S_{8}(24), S_{22}(10) \\ v(C.C_a)' & 1248.9 & 116.3 & S_{8}(25), S_{2}(43) \\ v(ring 5)' & 1163.1 & 4.5 & S_{9}(10), S_{13}(43), S_{33}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{9}(10), S_{13}(43), S_{33}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{9}(10), S_{13}(49), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_{9}(10), S_{13}(49), S_{34}(13) \\ v(ring 1) & 1105.9 & 24.7 & S_{6}(50), S_{7}(19) \\ \delta(C-H 13)' & 1088.4 & 26.5 & S_{7}(28), S_{13}(13), S_{13}(11) \\ \delta(C-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{34}(11), S_{17}(39) \\ \delta(C-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{34}(11), S_{17}(39) \\ \delta(C-H 3)' & 1018.5 & 83.1 & S_{12}(27), S_{34}(27) \\ \delta(ring 1)' & 938.3 & 11.5 & S_{11}(10), S_{29}(16) \\ \delta(ring 1)' & 938.3 & 11.5 & S_{11}(10), S_{29}(16) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{33}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{33}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{33}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{33}(56) \\ \delta(ring 1)' & 738.3 & 224.2 & S_{24}(19), S_{24}(12) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(C-H 1)' & 738.3 & 224.2 & S_{23}(19), S_{40}(13), S_{41}(23) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{29}(23), S_{40}(23), S_{40}(24) \\ v(ring 1)' & 590.4 & 14.7 & S_{29}(23), S_{40}(23), S_{40}(24) \\ v(ring 1)' & 590.4 & 14.7 & S_{29}(53), S_{40}(13) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{29}(53), S_{40}(13) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{29}(53), S_{40}(13) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{29}(53), S_{40}(13) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{29}(53), S_{40}(13) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{29}(53), S_{40}(14) \\ \delta(C-O)' & 489.5 & 2.8 & S_{2}(29), S_{20}(10), S_{20}(12), S_{20}(22), S_{20}(22) \\ \sigma(ring)' & 265.7 & 3.1 & S_{1}(13), S_{4}(17), S_{27}(23) \\ \sigma(ring)' & 264.7 & $	v(ring 3)	1562.3	63.4	$S_4(10), S_{10}(55)$
	v(ring 3)'	1554.9	54.7	$S_{11}(58), S_{35}(12)$
	v(ring 2)'	1456.9	60.2	$S_8(22), S_9(30), S_{34}(10)$
	v(ring 2)	1450.2	181.6	$S_8(27), S_9(29)$
	$\nu(ring 4)$	1394.5	37.1	$S_{13}(40), S_{33}(15), S_{34}(10)$
$ \begin{array}{cccccc} v(c-C_a)' & 1298.5 & 21.8 & S_1(12), S_4(24), S_{22}(10) \\ v(c-C_a)' & 1248.9 & 116.3 & S_5(26), S_6(17), S_7(14), S_{32}(15) \\ \delta(c-H 1)' & 1223.6 & 2.2 & S_3(66) \\ \delta(c-H 1)' & 1216.3 & 3.4 & S_{14}(25), S_{32}(43) \\ v(ring 5)' & 1163.1 & 4.5 & S_6(10), S_{15}(49), S_{34}(13) \\ v(ring 5)' & 1163.1 & 4.5 & S_6(10), S_{15}(49), S_{34}(13) \\ v(ring 1) & 1105.9 & 24.7 & S_6(50), S_7(19) \\ \delta(c-H 2)' & 1088.4 & 26.5 & S_7(28), S_{15}(13), S_{35}(11) \\ \delta(c-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{35}(11), S_{37}(39) \\ \delta(c-H 2)' & 1008.9 & 40.5 & S_{17}(27), S_{36}(27) \\ \delta(c-H 3)' & 1018.5 & 83.1 & S_{13}(28), S_{35}(11), S_{37}(39) \\ \delta(c-H 2)' & 1008.9 & 40.5 & S_{17}(27), S_{36}(24) \\ v(ring 1)' & 938.3 & 11.5 & S_7(11), S_{15}(10), S_{29}(16) \\ \delta(ring 1) & 905.9 & 13.2 & S_{28}(40) \\ \gamma(c-H 3)' & 884.9 & 1.7 & S_{53}(93) \\ \gamma(c-H 3)' & 884.9 & 1.4 & S_{54}(23), S_{36}(56) \\ \delta(ring 2)' & 883.3 & 14.9 & S_{29}(27), S_{31}(56) \\ \gamma(c-H 2)' & 840.7 & 6.5 & S_{52}(84) \\ \gamma(c-O)' & 811.9 & 51.3 & S_{21}(15), S_{43}(36), S_{51}(26) \\ \gamma(c-H 1)' & 760.8 & 76.7 & S_{68}(2) \\ \gamma(c-H 1)' & 760.8 & 76.7 & S_{68}(2) \\ \gamma(c-H 1)' & 760.8 & 76.7 & S_{68}(2) \\ \gamma(c-H 1)' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(c-H 1)' & 783.3 & 224.2 & S_{21}(19), S_{24}(22), S_{47}(29) \\ \tau(ring 2)' & 626.0 & 5.4 & S_{24}(10), S_{39}(11), S_{41}(53) \\ \tau(ring 1)' & 738.3 & 224.2 & S_{21}(9), S_{29}(12), S_{48}(22) \\ v(c-C)' & 718.2 & 9.9 & S_{1}(10), S_{30}(11), S_{41}(53) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{78}(85), S_{61}(18) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{78}(85), S_{61}(18) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{78}(85), S_{61}(18) \\ \tau(ring 1)' & 590.4 & 14.7 & S_{78}(85), S_{61}(13) \\ \sigma(ring)' & 265.5 & 3.1 & S_{1}(3), S_{61}(7), S_{27}(22) \\ \phi(ring)' & 285.5 & 3.1 & S_{1}(3), S_{61}(7), S_{27}(32) \\ \phi(ring)' & 285.5 & 3.1 & S_{1}(3), S_{61}(13), S_{62}(3) \\ \gamma(ring)' & 162.5 & 0.1 & S_{27}(16), S_{63}(3) \\ \gamma(ring)' & 162.5 & 0.1 & S_{27}(16), S_{63}(37) \\ \end{array}$	v(ring 4)	1390.2	19.5	$S_{12}(44), S_{32}(14), S_{35}(10)$
$v(C-C_a)^*$ 1248.9116.3 $S_5(26), S_6(17), S_7(14), S_{32}(15)$ $\delta(C-H 1)^*$ 1223.62.2 $S_{33}(66)$ $\delta(C-H 1)^*$ 1216.33.4 $S_{14}(25), S_{32}(43)$ $v(ring 5)^*$ 1163.14.5 $S_9(10), S_1(49), S_{34}(13)$ $v(ring 5)^*$ 1155.510.1 $S_8(23), S_1(43), S_{35}(13)$ $v(ring 1)^*$ 1105.924.7 $S_6(50), S_7(19)$ $\delta(C-H 2)^*$ 1088.426.5 $S_7(28), S_1(3), S_{35}(11)$ $\delta(C-H 3)^*$ 1018.583.1 $S_1(22), S_{36}(27)$ $\delta(C-H 3)^*$ 1018.583.1 $S_1(22), S_{36}(24)$ $v(ring 1)^*$ 938.311.5 $S_7(11), S_{37}(10), S_{39}(16)$ $\delta(C-H 2)^*$ 1008.940.5 $S_{12}(27), S_{34}(21), S_{36}(24)$ $v(ring 1)^*$ 938.311.5 $S_7(11), S_{15}(10), S_{29}(16)$ $\delta(ring 1)^*$ 905.913.2 $S_{28}(40)$ $v(C-H 3)^*$ 884.01.7 $S_{54}(98)$ $\delta(ring 2)^*$ 884.14.8 $S_{29}(27), S_{15}(56)$ $v(C-H 2)^*$ 840.76.5 $S_{52}(84)$ $v(C-H 2)^*$ 840.76.5 $S_{52}(84)$ $v(C-H 1)^*$ 760.876.7 $S_{50}(82)$ $v(C-H 1)^*$ 780.876.7 $S_{50}(82)$ $v(C-C)^*$ 718.29.9 $S_{1}(1), S_{3}(12)$ $v(C-C)^*$ 718.29.9 $S_{1}(1), S_{3}(11), S_{4}(53)$ $v(ring 1)^*$ 590.414.7 $S_{39}(83), S_{41}(18)$ $v(ring 1)^*$ 590.414.7 $S_{39}(21), S_{30}(10)$	$v(C-C_{\alpha})$	1298.5	21.8	$S_1(12), S_4(24), S_{22}(10)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$\nu(C-C_{\alpha})$	1248.9	116.3	$S_5(26), S_6(17), S_7(14), S_{32}(15)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	δ(C-H 1)'	1223.6	2.2	S ₃₃ (66)
v(ring 5)'1163.14.5 $S_9(10), S_{15}(49), S_{34}(13)$ v(ring 5)1155.510.1 $S_8(23), S_{14}(33), S_{53}(13)$ v(ring 1)1105.924.7 $S_6(50), S_7(19)$ $\delta(C-H 2)'$ 1088.426.5 $S_7(28), S_{15}(13), S_{15}(11)$ $\delta(C-H 3)$ 1058.93.7 $S_1(12), S_{36}(27)$ $\delta(C-H 3)'$ 1018.583.1 $S_{12}(28), S_{35}(11), S_{36}(24)$ $v(ring 1)'$ 938.311.5 $S_{711}, S_{15}(10), S_{29}(16)$ $\delta(ring 1)$ 905.913.2 $S_{28}(40)$ $v(ring 1)'$ 988.91.4 $S_{54}(98)$ $\delta(ring 2)'$ 884.14.8 $S_{32}(27), S_{31}(56)$ $v(C-H 3)'$ 849.27.4 $S_{48}(15), S_{51}(57), S_{53}(12)$ $\delta(ring 2)'$ 843.314.9 $S_{29}(27), S_{31}(56)$ $v(C-H 2)'$ 840.76.5 $S_{52}(84)$ $v(C-H 1)'$ 760.876.7 $S_{50}(82)$ $v(C-H 1)'$ 760.876.7 $S_{50}(25)$ $v(C-C)'$ 718.29.9 $S_{11}(1), S_{14}(15)$ $v(ring 1)'$ 738.3224.2 $S_{24}(10), S_{39}(11), S_{41}(53)$ $v(ring 2)'$ 626.05.4 $S_{24}(10), S_{39}(11), S_{41}(53)$ $v(ring 1)'$ 590.41.4.7 $S_{36}(5), S_{41}(18)$ $v(ring 1)'$ 590.41.4.7 $S_{36}(5), S_{41}(18)$ $v(C-C)'$ 718.29.9 $S_{12}(2), S_{22}(1), S_{22}(10)$ $v(C-C)'$ 718.29.9 $S_{12}(2), S_{22}(1), S_{23}(10)$ $v(C-C)'$ 489.52.8	δ(C-H 1)	1216.3	3.4	$S_{14}(25), S_{32}(43)$
	v(ring 5)'	1163.1	4.5	$S_9(10), S_{15}(49), S_{34}(13)$
v(ring 1)1105.924.7 $S_6(50), S_7(19)$ $\delta(C-H 2)'$ 1088.426.5 $S_7(28), S_{15}(13), S_{35}(11)$ $\delta(C-H 3)'$ 1058.93.7 $S_{1}(12), S_{36}(27)$ $\delta(C-H 3)'$ 1018.583.1 $S_{12}(28), S_{35}(11), S_{37}(39)$ $\delta(C-H 2)'$ 1008.940.5 $S_{12}(27), S_{34}(21), S_{36}(24)$ $v(ring 1)'$ 938.311.5 $S_{7}(11), S_{15}(10), S_{29}(16)$ $\delta(ring 1)'$ 905.913.2 $S_{28}(40)$ $\gamma(C-H 3)'$ 884.01.7 $S_{53}(93)$ $\gamma(C-H 3)'$ 888.91.4 $S_{54}(98)$ $\delta(ring 2)'$ 884.14.8 $S_{26}(23), S_{30}(56)$ $\delta(ring 2)'$ 883.314.9 $S_{29}(27), S_{31}(56)$ $\gamma(C-H 2)'$ 840.76.5 $S_{25}(84)$ $\gamma(C-H 2)'$ 840.76.5 $S_{25}(84)$ $\gamma(C-H 1)'$ 760.87.7 $S_{50}(82)$ $\gamma(C-H 1)'$ 760.87.7 $S_{50}(82)$ $\gamma(C-H 1)'$ 759.345.3 $S_{49}(81)$ $\delta(ring 1)'$ 783.3224.2 $S_{21}(19), S_{29}(12), S_{48}(22)$ $v(C-C)'$ 718.29.9 $S_{1}(10), S_{24}(22), S_{47}(29)$ $t(ring 2)'$ 626.05.4 $S_{24}(10), S_{39}(11), S_{41}(53)$ $t(ring 1)'$ 590.414.7 $S_{38}(85), S_{41}(18)$ $t(ring 1)'$ 590.414.7 $S_{38}(85), S_{41}(18)$ $t(ring 1)'$ 590.414.7 $S_{32}(36), S_{22}(14), S_{26}(31), S_{29}(10)$ $t(ring 1)'$ 590.414.7 $S_{32}(36), S_{32}(14$	v(ring 5)	1155.5	10.1	$S_8(23), S_{14}(33), S_{35}(13)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	v(ring 1)	1105.9	24.7	$S_6(50), S_7(19)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	δ(С-Н 2)'	1088.4	26.5	$S_7(28), S_{15}(13), S_{35}(11)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	δ(С-Н 3)	1058.9	3.7	$S_1(12), S_{36}(27)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	δ(С-Н 3)'	1018.5	83.1	$S_{13}(28), S_{35}(11), S_{37}(39)$
v(ring 1)'938.311.5 $S_7(11), S_{15}(10), S_{29}(16)$ δ (ring 1)905.913.2 $S_{28}(40)$ γ (C-H 3)894.01.7 $S_{53}(93)$ γ (C-H 3)'888.91.4 $S_{54}(98)$ δ (ring 2)884.14.8 $S_{28}(23), S_{30}(56)$ δ (ring 2)'883.314.9 $S_{29}(27), S_{31}(56)$ γ (C-H 2)849.27.4 $S_{48}(15), S_{51}(57), S_{53}(12)$ γ (C-H 2)'840.76.5 $S_{52}(84)$ γ (C-H 1)'760.876.7 $S_{50}(82)$ γ (C-H 1)759.345.3 $S_{49}(81)$ δ (ring 1)'738.3224.2 $S_{23}(19), S_{29}(12), S_{48}(22)$ ν (C-C)718.29.9 $S_{1}(10), S_{24}(22), S_{47}(29)$ τ (ring 2)'618.52.1 $S_{40}(75)$ τ (ring 1)'590.41.4.7 $S_{39}(85), S_{41}(18)$ τ (ring 1)'590.41.4.7 $S_{39}(85), S_{41}(18)$ τ (ring 1)'590.41.4.7 $S_{39}(35), S_{40}(11)$ δ (C=O)'489.52.8 $S_{5}(29), S_{23}(16), S_{29}(10), S_{29}(10)$ γ (C=O)475.88.0 $S_{4}(23), S_{47}(24)$ δ (C=O)342.93.5 $S_{1}(29), S_{22}(52)$ ω (ring)'285.53.1 $S_{1}(13), S_{4}(17), S_{27}(32)$ ω (ring)'264.724.3 $S_{23}(36), S_{25}(14), S_{26}(3)$ γ (ring)'162.50.1 $S_{27}(16), S_{43}(50)$ δ (CCC $_{\alpha}$)149.81.3 $S_{23}(24), S_{27}(21), S_{43}(11), S_{$	δ(C-H 2)	1008.9	40.5	$S_{12}(27), S_{34}(21), S_{36}(24)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	v(ring 1)'	938.3	11.5	$S_7(11), S_{15}(10), S_{29}(16)$
$\begin{array}{cccccc} \gamma(\text{C-H 3}) & 894.0 & 1.7 & \text{S}_{53}(93) \\ \gamma(\text{C-H 3})' & 888.9 & 1.4 & \text{S}_{54}(98) \\ \delta(\text{ring 2}) & 884.1 & 4.8 & \text{S}_{28}(23), \text{S}_{30}(56) \\ \delta(\text{ring 2})' & 883.3 & 14.9 & \text{S}_{29}(27), \text{S}_{31}(56) \\ \gamma(\text{C-H 2}) & 849.2 & 7.4 & \text{S}_{48}(15), \text{S}_{51}(57), \text{S}_{53}(12) \\ \gamma(\text{C-H 2})' & 840.7 & 6.5 & \text{S}_{22}(84) \\ \gamma(\text{C=O})' & 811.9 & 51.3 & \text{S}_{23}(15), \text{S}_{48}(36), \text{S}_{51}(26) \\ \gamma(\text{C-H 1})' & 760.8 & 76.7 & \text{S}_{50}(82) \\ \gamma(\text{C-H 1}) & 759.3 & 45.3 & \text{S}_{49}(81) \\ \delta(\text{ring 1})' & 738.3 & 224.2 & \text{S}_{23}(19), \text{S}_{29}(12), \text{S}_{48}(22) \\ \nu(\text{C-C}) & 718.2 & 9.9 & \text{S}_{1}(10), \text{S}_{24}(22), \text{S}_{47}(29) \\ \tau(\text{ring 2})' & 626.0 & 5.4 & \text{S}_{24}(10), \text{S}_{39}(11), \text{S}_{41}(53) \\ \tau(\text{ring 1})' & 590.4 & 14.7 & \text{S}_{39}(85), \text{S}_{41}(18) \\ \tau(\text{ring 1}) & 588.9 & 2.3 & \text{S}_{38}(93), \text{S}_{40}(11) \\ \delta(\text{C=O})' & 489.5 & 2.8 & \text{S}_{5}(29), \text{S}_{23}(16), \text{S}_{29}(10) \\ \gamma(\text{C=O}) & 475.8 & 8.0 & \text{S}_{4}(23), \text{S}_{47}(24) \\ \delta(\text{C=O})' & 342.9 & 3.5 & \text{S}_{1}(29), \text{S}_{22}(52) \\ \omega(\text{ring})' & 285.5 & 3.1 & \text{S}_{1}(13), \text{S}_{4}(17), \text{S}_{27}(32) \\ \omega(\text{ring}) & 174.1 & 0.2 & \text{S}_{42}(63), \text{S}_{43}(12) \\ \gamma(\text{ring})' & 162.5 & 0.1 & \text{S}_{27}(16), \text{S}_{43}(50) \\ \delta(\text{CCC}_{\alpha}) & 149.8 & 1.3 & \text{S}_{24}(34), \text{S}_{27}(21), \text{S}_{43}(11), \text{S}_{44}(12), \text{S}_{47}(12) \\ \delta(\text{CCC}_{\alpha})' & 125.3 & 0.7 & \text{S}_{2}(56), \text{S}_{6}(21), \text{S}_{46}(37) \\ \end{array}$	δ(ring 1)	905.9	13.2	S ₂₈ (40)
$\begin{array}{cccccc} \gamma(\text{C-H 3})' & 888.9 & 1.4 & \text{S}_{54}(98) \\ \hline \delta(\text{ring 2}) & 884.1 & 4.8 & \text{S}_{28}(23), \text{S}_{30}(56) \\ \hline \delta(\text{ring 2})' & 883.3 & 14.9 & \text{S}_{29}(27), \text{S}_{31}(56) \\ \gamma(\text{C-H 2}) & 849.2 & 7.4 & \text{S}_{48}(15), \text{S}_{51}(57), \text{S}_{53}(12) \\ \gamma(\text{C-H 2})' & 840.7 & 6.5 & \text{S}_{52}(84) \\ \gamma(\text{C-O})' & 811.9 & 51.3 & \text{S}_{23}(15), \text{S}_{48}(36), \text{S}_{51}(26) \\ \gamma(\text{C-H 1})' & 760.8 & 76.7 & \text{S}_{60}(82) \\ \gamma(\text{C-H 1}) & 759.3 & 45.3 & \text{S}_{49}(81) \\ \hline \delta(\text{ring 1})' & 738.3 & 224.2 & \text{S}_{23}(19), \text{S}_{29}(12), \text{S}_{48}(22) \\ \nu(\text{C-C}) & 718.2 & 9.9 & \text{S}_{1}(10), \text{S}_{24}(22), \text{S}_{47}(29) \\ \tau(\text{ring 2})' & 626.0 & 5.4 & \text{S}_{24}(10), \text{S}_{39}(11), \text{S}_{41}(53) \\ \tau(\text{ring 1})' & 590.4 & 14.7 & \text{S}_{39}(85), \text{S}_{41}(18) \\ \tau(\text{ring 1}) & 588.9 & 2.3 & \text{S}_{38}(93), \text{S}_{40}(11) \\ \delta(\text{C=O})' & 489.5 & 2.8 & \text{S}_{2}(29), \text{S}_{23}(16), \text{S}_{29}(10) \\ \gamma(\text{C=O}) & 475.8 & 8.0 & \text{S}_{4}(23), \text{S}_{47}(24) \\ \delta(\text{C=O}) & 342.9 & 3.5 & \text{S}_{1}(29), \text{S}_{2}(52) \\ \omega(\text{ring})' & 285.5 & 3.1 & \text{S}_{1}(13), \text{S}_{4}(17), \text{S}_{2}(32) \\ \omega(\text{ring})' & 264.7 & 24.3 & \text{S}_{23}(63), \text{S}_{34}(12) \\ \gamma(\text{ring})' & 162.5 & 0.1 & \text{S}_{27}(16), \text{S}_{43}(50) \\ \delta(\text{CCC}_{\alpha})' & 125.3 & 0.7 & \text{S}_{2}(54), \text{S}_{26}(21), \text{S}_{46}(37) \\ \end{array}$	γ(C-H 3)	894.0	1.7	S ₅₃ (93)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	γ(C-H 3)'	888.9	1.4	S ₅₄ (98)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	$\delta(ring 2)$	884.1	4.8	$S_{28}(23), S_{30}(56)$
$\begin{array}{cccccc} \gamma(\text{C-H 2}) & 849.2 & 7.4 & S_{48}(15), S_{51}(57), S_{53}(12) \\ \gamma(\text{C-H 2})' & 840.7 & 6.5 & S_{52}(84) \\ \gamma(\text{C=O})' & 811.9 & 51.3 & S_{23}(15), S_{48}(36), S_{51}(26) \\ \gamma(\text{C-H 1})' & 760.8 & 76.7 & S_{50}(82) \\ \gamma(\text{C-H 1}) & 759.3 & 45.3 & S_{49}(81) \\ \delta(\text{ring 1})' & 738.3 & 224.2 & S_{23}(19), S_{29}(12), S_{48}(22) \\ \nu(\text{C-C}) & 718.2 & 9.9 & S_{1}(10), S_{24}(22), S_{47}(29) \\ \tau(\text{ring 2})' & 626.0 & 5.4 & S_{24}(10), S_{39}(11), S_{41}(53) \\ \tau(\text{ring 1})' & 590.4 & 14.7 & S_{39}(85), S_{41}(18) \\ \tau(\text{ring 1}) & 588.9 & 2.3 & S_{38}(93), S_{40}(11) \\ \delta(\text{C=O})' & 489.5 & 2.8 & S_{5}(29), S_{23}(16), S_{26}(13), S_{29}(10) \\ \gamma(\text{C=O}) & 475.8 & 8.0 & S_{4}(23), S_{47}(24) \\ \delta(\text{C=O}) & 342.9 & 3.5 & S_{1}(29), S_{22}(52) \\ \omega(\text{ring})' & 285.5 & 3.1 & S_{1}(13), S_{4}(17), S_{27}(32) \\ \omega(\text{ring}) & 174.1 & 0.2 & S_{42}(63), S_{43}(11), S_{44}(12), S_{47}(12) \\ \gamma(\text{ring})' & 162.5 & 0.1 & S_{27}(16), S_{43}(11), S_{44}(12), S_{47}(12) \\ \delta(\text{CCC}_{a}) & 149.8 & 1.3 & S_{24}(34), S_{27}(21), S_{46}(37) \\ \end{array}$	δ(ring 2)'	883.3	14.9	$S_{29}(27), S_{31}(56)$
$\gamma(C-H 2)'$ 840.76.5 $S_{52}(84)$ $\gamma(C=O)'$ 811.951.3 $S_{23}(15), S_{48}(36), S_{51}(26)$ $\gamma(C-H 1)'$ 760.876.7 $S_{50}(82)$ $\gamma(C-H 1)$ 759.345.3 $S_{49}(81)$ $\delta(ring 1)'$ 738.3224.2 $S_{23}(19), S_{29}(12), S_{48}(22)$ $\nu(C-C)$ 718.29.9 $S_1(10), S_{24}(22), S_{47}(29)$ $\tau(ring 2)'$ 626.05.4 $S_{24}(10), S_{39}(11), S_{41}(53)$ $\tau(ring 1)'$ 590.414.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)'$ 590.414.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)'$ 590.414.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)'$ 588.92.3 $S_{38}(93), S_{40}(11)$ $\delta(C=O)'$ 475.88.0 $S_4(23), S_{47}(24)$ $\delta(C=O)$ 342.93.5 $S_{1}(29), S_{22}(52)$ $\omega(ring)'$ 285.53.1 $S_{1}(13), S_{4}(17), S_{27}(32)$ $\omega(ring)'$ 264.724.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)'$ 162.50.1 $S_{27}(16), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})$ 149.81.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.30.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	γ(C-H 2)	849.2	7.4	$S_{48}(15), S_{51}(57), S_{53}(12)$
$\gamma(C=O)'$ 811.9 51.3 $S_{23}(15), S_{48}(36), S_{51}(26)$ $\gamma(C-H 1)'$ 760.8 76.7 $S_{50}(82)$ $\gamma(C-H 1)$ 759.3 45.3 $S_{49}(81)$ $\delta(ring 1)'$ 738.3 224.2 $S_{23}(19), S_{29}(12), S_{48}(22)$ $\nu(C-C)$ 718.2 9.9 $S_1(10), S_{24}(22), S_{47}(29)$ $\tau(ring 2)'$ 626.0 5.4 $S_{24}(10), S_{39}(11), S_{41}(53)$ $\tau(ring 1)'$ 590.4 14.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)'$ 588.9 2.3 $S_{38}(93), S_{40}(11)$ $\delta(C=O)'$ 489.5 2.8 $S_{5}(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.8 8.0 $S_{4}(23), S_{47}(24)$ $\delta(C=O)$ 342.9 3.5 $S_{1}(29), S_{22}(52)$ $\omega(ring)'$ 285.5 3.1 $S_{1}(13), S_{4}(17), S_{27}(32)$ $\omega(ring)'$ 264.7 24.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)'$ 162.5 0.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.8 1.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.3 0.7 $S_{25}(36), S_{26}(21), S_{46}($	γ(C-H 2)'	840.7	6.5	S ₅₂ (84)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	γ(C=O)'	811.9	51.3	$S_{23}(15), S_{48}(36), S_{51}(26)$
$\begin{array}{cccccc} \gamma(\text{C-H 1}) & 759.3 & 45.3 & \text{S}_{49}(81) \\ \hline \delta(\text{ring 1})' & 738.3 & 224.2 & \text{S}_{23}(19), \text{S}_{29}(12), \text{S}_{48}(22) \\ \nu(\text{C-C}) & 718.2 & 9.9 & \text{S}_1(10), \text{S}_{24}(22), \text{S}_{47}(29) \\ \hline \tau(\text{ring 2})' & 626.0 & 5.4 & \text{S}_{24}(10), \text{S}_{39}(11), \text{S}_{41}(53) \\ \hline \tau(\text{ring 2}) & 618.5 & 2.1 & \text{S}_{40}(75) \\ \hline \tau(\text{ring 1})' & 590.4 & 14.7 & \text{S}_{39}(85), \text{S}_{41}(18) \\ \hline \tau(\text{ring 1}) & 588.9 & 2.3 & \text{S}_{38}(93), \text{S}_{40}(11) \\ \delta(\text{C=O})' & 489.5 & 2.8 & \text{S}_5(29), \text{S}_{23}(16), \text{S}_{26}(13), \text{S}_{29}(10) \\ \gamma(\text{C=O}) & 475.8 & 8.0 & \text{S}_4(23), \text{S}_{47}(24) \\ \delta(\text{C=O}) & 342.9 & 3.5 & \text{S}_1(29), \text{S}_{22}(52) \\ \omega(\text{ring})' & 285.5 & 3.1 & \text{S}_1(13), \text{S}_4(17), \text{S}_{27}(32) \\ \omega(\text{ring}) & 264.7 & 24.3 & \text{S}_{23}(36), \text{S}_{25}(14), \text{S}_{26}(33) \\ \gamma(\text{ring}) & 174.1 & 0.2 & \text{S}_{42}(63), \text{S}_{43}(12) \\ \gamma(\text{ring})' & 162.5 & 0.1 & \text{S}_{27}(16), \text{S}_{43}(50) \\ \delta(\text{CCC}_{\alpha}) & 149.8 & 1.3 & \text{S}_{24}(34), \text{S}_{27}(21), \text{S}_{43}(11), \text{S}_{44}(12), \text{S}_{47}(12) \\ \delta(\text{CCC}_{\alpha})' & 125.3 & 0.7 & \text{S}_{25}(36), \text{S}_{26}(21), \text{S}_{46}(37) \end{array}$	γ(C-H 1) ²	760.8	76.7	$S_{50}(82)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	γ(C-H 1)	759.3	45.3	$S_{49}(81)$
$v(C-C)$ 718.2 9.9 $S_1(10), S_{24}(22), S_{47}(29)$ $\tau(ring 2)$ ' 626.0 5.4 $S_{24}(10), S_{39}(11), S_{41}(53)$ $\tau(ring 2)$ 618.5 2.1 $S_{40}(75)$ $\tau(ring 1)$ ' 590.4 14.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)$ 588.9 2.3 $S_{38}(93), S_{40}(11)$ $\delta(C=O)$ ' 489.5 2.8 $S_5(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.8 8.0 $S_4(23), S_{47}(24)$ $\delta(C=O)$ 342.9 3.5 $S_1(29), S_{22}(52)$ $\omega(ring)$ ' 285.5 3.1 $S_1(13), S_4(17), S_{27}(32)$ $\omega(ring)$ 264.7 24.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ ' 174.1 0.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)$ ' 162.5 0.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.8 1.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})$ ' 125.3 0.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	$\delta(\operatorname{ring} 1)'$	738.3	224.2	$S_{23}(19), S_{29}(12), S_{48}(22)$
$\tau(ring 2)'$ 626.05.4 $S_{24}(10), S_{39}(11), S_{41}(53)$ $\tau(ring 2)$ 618.52.1 $S_{40}(75)$ $\tau(ring 1)'$ 590.414.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)$ 588.92.3 $S_{38}(93), S_{40}(11)$ $\delta(C=O)'$ 489.52.8 $S_5(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.88.0 $S_4(23), S_{47}(24)$ $\delta(C=O)$ 342.93.5 $S_1(29), S_{22}(52)$ $\omega(ring)'$ 285.53.1 $S_1(13), S_4(17), S_{27}(32)$ $\omega(ring)$ 264.724.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ 174.10.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)'$ 162.50.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.81.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.30.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	v(C-C)	718.2	9.9	$S_1(10), S_{24}(22), S_{47}(29)$
$\tau(ring 2)$ 618.52.1 $S_{40}(75)$ $\tau(ring 1)'$ 590.414.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)$ 588.92.3 $S_{38}(93), S_{40}(11)$ $\delta(C=O)'$ 489.52.8 $S_5(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.88.0 $S_4(23), S_{47}(24)$ $\delta(C=O)$ 342.93.5 $S_1(29), S_{22}(52)$ $\omega(ring)'$ 285.53.1 $S_1(13), S_4(17), S_{27}(32)$ $\omega(ring)$ 264.724.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ 174.10.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)'$ 162.50.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.81.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.30.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	$\tau(\operatorname{ring} 2)$	626.0	5.4	$S_{24}(10), S_{39}(11), S_{41}(53)$
$\tau(ring 1)^{\prime}$ 590.414.7 $S_{39}(85), S_{41}(18)$ $\tau(ring 1)$ 588.92.3 $S_{38}(93), S_{40}(11)$ $\delta(C=O)^{\prime}$ 489.52.8 $S_{5}(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.88.0 $S_{4}(23), S_{47}(24)$ $\delta(C=O)$ 342.93.5 $S_{1}(29), S_{22}(52)$ $\omega(ring)^{\prime}$ 285.53.1 $S_{1}(13), S_{4}(17), S_{27}(32)$ $\omega(ring)$ 264.724.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ 174.10.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)^{\prime}$ 162.50.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.81.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})^{\prime}$ 125.30.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	$\tau(\operatorname{ring} 2)$	618.5	2.1	$S_{40}(75)$
$\tau(ring 1)$ 588.92.3 $S_{38}(95), S_{40}(11)$ $\delta(C=O)'$ 489.52.8 $S_5(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.88.0 $S_4(23), S_{47}(24)$ $\delta(C=O)$ 342.93.5 $S_1(29), S_{22}(52)$ $\omega(ring)'$ 285.53.1 $S_1(13), S_4(17), S_{27}(32)$ $\omega(ring)$ 264.724.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ 174.10.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)'$ 162.50.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.81.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.30.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	$\tau(\operatorname{ring} 1)$	590.4	14./	$S_{39}(85), S_{41}(18)$
$\delta(C=O)$ 489.5 2.8 $S_5(29), S_{23}(16), S_{26}(13), S_{29}(10)$ $\gamma(C=O)$ 475.8 8.0 $S_4(23), S_{47}(24)$ $\delta(C=O)$ 342.9 3.5 $S_1(29), S_{22}(52)$ $\omega(ring)'$ 285.5 3.1 $S_1(13), S_4(17), S_{27}(32)$ $\omega(ring)$ 264.7 24.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ 174.1 0.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)'$ 162.5 0.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.8 1.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.3 0.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	$\tau(\text{ring I})$	588.9	2.3	$S_{38}(93), S_{40}(11)$
$\begin{array}{llllllllllllllllllllllllllllllllllll$	8(C=O)	489.5	2.8	$S_{5}(29), S_{23}(10), S_{26}(15), S_{29}(10)$
$o(C=O)$ 542.9 5.5 $S_{1}(29), S_{22}(32)$ $\omega(ring)'$ 285.5 3.1 $S_{1}(13), S_{4}(17), S_{27}(32)$ $\omega(ring)$ 264.7 24.3 $S_{23}(36), S_{25}(14), S_{26}(33)$ $\gamma(ring)$ 174.1 0.2 $S_{42}(63), S_{43}(12)$ $\gamma(ring)'$ 162.5 0.1 $S_{27}(16), S_{43}(50)$ $\delta(CCC_{\alpha})$ 149.8 1.3 $S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $\delta(CCC_{\alpha})'$ 125.3 0.7 $S_{25}(36), S_{26}(21), S_{46}(37)$	$\gamma(C=O)$	4/5.8	8.0	$S_4(25), S_{47}(24)$ $S_5(20), S_{5}(52)$
$\begin{array}{ccccccc} \omega(ring) & 283.5 & 5.1 & S_1(13), S_4(17), S_{27}(32) \\ \omega(ring) & 264.7 & 24.3 & S_{23}(36), S_{25}(14), S_{26}(33) \\ \gamma(ring) & 174.1 & 0.2 & S_{42}(63), S_{43}(12) \\ \gamma(ring)' & 162.5 & 0.1 & S_{27}(16), S_{43}(50) \\ \delta(CCC_{\alpha}) & 149.8 & 1.3 & S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12) \\ \delta(CCC_{\alpha})' & 125.3 & 0.7 & S_{25}(36), S_{26}(21), S_{46}(37) \end{array}$	O(C=O)	342.9	3.5	$S_1(29), S_{22}(52)$ $S_1(12), S_2(17), S_2(22)$
$\begin{array}{ccccccc} & & & & & & & & & & & & & & & &$	$\omega(\text{ring})$	285.5	3.1 24.2	$S_1(15), S_4(17), S_{27}(52)$ $S_1(26), S_1(14), S_2(32)$
$\begin{array}{cccc} \gamma(\mathrm{ring}) & 1.74.1 & 0.2 & 34_2(03), 54_3(12) \\ \gamma(\mathrm{ring})' & 162.5 & 0.1 & S_{27}(16), S_{43}(50) \\ \delta(\mathrm{CCC}_{\alpha}) & 149.8 & 1.3 & S_{24}(34), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12) \\ \delta(\mathrm{CCC}_{\alpha})' & 125.3 & 0.7 & S_{25}(36), S_{26}(21), S_{46}(37) \end{array}$	w(ring)	204.7 1771	24.5	$S_{23}(50), S_{25}(14), S_{26}(55)$ $S_{10}(63), S_{10}(12)$
$\begin{array}{cccc} & & & & & & & & & & & & & & & & & $	y(ring)	1/4.1	0.2	$S_{42}(05), S_{43}(12)$ $S_{57}(16), S_{59}(50)$
$\delta(\text{CCC}_{\alpha})^{\prime} \qquad 125.3 \qquad 1.5 3_{24}(3+), 3_{27}(2+), 3_{33}(1+), 3_{44}(12), 3_{47}(12)$	$\gamma(\text{rmg})$	102.3	0.1	$S_{2/(10)}, S_{43}(50)$ $S_{2/(10)}, S_{3}(21), S_{3}(11), S_{3}(12), S_{3}(12)$
0.7 0.25(50), 0.26(21), 0.46(57)	$\delta(CCC_{\alpha})$	177.0	1.5	$S_{24}(51), S_{27}(21), S_{43}(11), S_{44}(12), S_{47}(12)$ $S_{25}(36), S_{25}(21), S_{45}(37)$
$\tau(C_{-}C_{-})'$ 62.3 2.0 $S_{-r}(21)$ $S_{+r}(59)$	$\tau(C-C)$	623	2.0	$S_{25}(35), S_{20}(21), S_{40}(57)$ $S_{55}(21), S_{40}(59)$
$\tau(C-C_{\alpha})$ 55.5 0.4 $S_{cc}(82)$	$\tau(C-C_{\alpha})$	55 5	2.0	$S_{25}(21), S_{46}(57)$ $S_{45}(82)$
$\tau(C-C)$ 25.7 5.0 $S_{AA}(87)$	$\tau(C-C)$	25 7	5.0	$S_{44}(87)$

Table S4- Calculated [scaled, DFT(B3LYP)/6-311++G(d,p)] wavenumbers, IR intensities and Potential Energy Distributions (PED) for conformer II of α -furil.^a

^a Wavenumbers in cm⁻¹, calculated intensities in km mol⁻¹, v, bond stretching, δ , bending, γ , rocking, ω ,

wagging, τ , torsion. See Table S2 for definition of internal coordinates and Figure 1 for atom numbering. ^b Scaled (0.978). ^c Only PED values greater than 10 % are given.

Approximate description	Wavenumber ^b	Intensity	PED ^c
v(C-H 1) as	3203.5	< 0.1	S ₁₇ (76), S ₁₉ (22)
v(C-H 1) s	3203.5	< 0.1	$S_{16}(76), S_{18}(22)$
v(C-H 2) s	3190.8	0.6	$S_{16}(22), S_{18}(77)$
v(C-H 2) as	3190.7	1.8	S ₁₇ (22), S ₁₉ (77)
v(C-H 3) s	3175.9	0.3	$S_{20}(99)$
ν (C-H 3) as	3175.9	1.2	$S_{21}(99)$
v(C=O) s	1692.5	183.9	S ₂ (90)
v(C=O) as	1683.1	345.9	S ₃ (95)
v(ring 3) s	1568.2	36.6	$S_4(14), S_{10}(62), S_{34}(10)$
v(ring 3) as	1562.8	146.3	$S_5(10), S_{11}(66), S_{35}(12)$
v(ring 2) s	1459.1	90.3	$S_4(10), S_8(47), S_{34}(12)$
v(ring 2) as	1452.6	185.9	$S_9(54), S_{35}(11)$
v(ring 4) s	1388.7	4.5	$S_{12}(44), S_{32}(15), S_{34}(18), S_{36}(11)$
v(ring 4) as	1387.5	17.8	$S_{13}(44), S_{33}(14), S_{35}(18), S_{37}(12)$
$v(C-C_{\alpha})$ s	1286.3	2.6	$S_1(12), S_4(23), S_6(11), S_8(16), S_{32}(18)$
$v(C-C_{\alpha})$ as	1243.1	123.1	$S_5(21), S_7(28), S_{33}(34)$
δ(C-H 1) s	1216.5	3.0	S ₁₄ (23), S ₃₂ (48)
δ(C-H 1) as	1211.2	10.1	$S_{15}(28), S_{33}(32)$
v(ring 5) s	1155.4	0.1	$S_8(22), S_{14}(35), S_{34}(18), S_{36}(13)$
v(ring 5) as	1153.6	25.3	$S_9(24), S_{15}(33), S_{35}(18), S_{37}(13)$
v(ring 1) s	1109.5	19.6	$S_{6}(71)$
v(ring 1) as	1088.3	33.2	$S_7(40), S_{15}(15), S_{35}(10), S_{37}(11)$
δ(C-H 3) s	1052.4	0.1	$S_1(13), S_{10}(14), S_{14}(15), S_{36}(24)$
δ(C-H 3) as	1011.8	104.0	$S_{13}(31), S_{35}(18), S_{37}(45)$
δ(C-H 2) s	1008.2	1.5	$S_{12}(30), S_{34}(28), S_{36}(30)$
δ(C-H 2) as	946.6	9.4	$S_7(15), S_{11}(10), S_{15}(15), S_{29}(15), S_{35}(11)$
$\delta(ring 1) s$	900.5	0.1	$S_{14}(12), S_{28}(33), S_{30}(21)$
γ (C-H 3) as	892.7	1.3	S ₅₂ (11), S ₅₄ (95)
γ(C-H 3) s	891.9	1.4	S ₅₁ (10), S ₅₃ (97)
$\delta(ring 2)$ as	883.4	12.7	$S_{29}(28), S_{31}(61)$
$\delta(ring 2) s$	883.1	1.3	$S_{28}(36), S_{30}(53)$
γ (C-H 2) as	847.4	20.5	$S_{48}(13), S_{52}(54), S_{54}(18)$
γ(C-H 2) s	840.4	4.4	$S_{51}(78), S_{53}(16)$
γ (C=O) as	813.4	76.4	$S_{23}(20), S_{29}(12), S_{48}(25), S_{52}(27)$
γ(C-H 1) s	758.3	74.1	$S_{49}(84), S_{51}(12)$
γ (C-H 1) as	757.8	45.3	$S_{50}(86), S_{52}(11)$
v(C-C)	739.8	16.3	$S_1(10), S_{24}(22), S_{47}(38)$
$\delta(ring 1)$ as	717.3	203.6	$S_{23}(13), S_{25}(11), S_{29}(11), S_{48}(27)$
$\tau(\text{ring 2})$ as	619.1	3.6	$S_{41}(82)$
$\tau(ring 2)$ s	618.9	4.9	S ₄₀ (79)
τ(ring 1) s	590.8	9.9	$S_{38}(95), S_{40}(12)$
τ(ring 1) as	589.3	3.7	S ₃₉ (99)
γ(C=O) s	483.1	4.1	$S_4(30), S_{47}(16)$
δ (C=O) as	481.9	1.4	$S_5(29), S_{23}(15), S_{27}(13)$
δ (C=O) s	329.8	2.9	$S_1(39), S_{22}(43)$
ω(ring) s	283.0	2.4	$S_4(13), S_{22}(17), S_{26}(32)$
$\omega(ring)$ as	261.8	30.4	$S_{23}(35), S_{25}(11), S_{27}(31)$
$\gamma(ring)$ as	173.9	0.3	$S_{43}(73)$
$\gamma(ring)$ s	167.6	0.1	$S_{42}(75)$
$\delta(CCC_{\alpha})$ s	126.2	0.9	$S_{24}(44), S_{26}(34)$
$\delta(CCC_{\alpha})$ as	122.1	0.1	$S_{25}(36), S_{27}(24), S_{46}(36)$
$\tau(C-C_{\alpha})$ s	58.2	0.6	$S_{45}(86)$
$\tau(C-C_{\alpha})$ as	56.3	2.2	$S_{25}(21), S_{46}(60)$
τ(C-C)	21.8	3.6	S ₄₄ (90)

Table S5- Calculated [scaled, DFT(B3LYP)/6-311++G(d,p)] wavenumbers, IR intensities and Potential Energy Distributions (PED) for conformer III of α -furil.^a

^a Wavenumbers in cm⁻¹, calculated intensities in km mol⁻¹, v, bond stretching, δ , bending, γ , rocking, ω ,

wagging, τ , torsion, s, symmetric, as, asymmetric. See Table S1 for definition of internal coordinates and Figure 1 for atom numbering. ^b Scaled (0.978). ^c Only PED values greater than 10 % are given.