Supplementary Material

Table 1S. Geometry of PTD conformers calculated at B3LYP/6-311++G(d,p) level (bond lengths in Å, angles in degrees; see Figure 2 for numbering of atoms).

Parameter	**Conformer**							
	I	**II**	**III**	**IV**	**V**	**VI**	**VII**	**VIII**
C_1-C_2	1.377	1.378	1.379	1.379	1.376	1.376	1.377	1.378
C_1-C_4	1.444	1.444	1.442	1.442	1.443	1.443	1.440	1.440
C_1-C_{19}	1.472	1.472	1.472	1.472	1.472	1.473	1.472	1.472
C_2-N_3	1.378	1.377	1.380	1.380	1.377	1.377	1.380	1.379
C_2-C_6	1.486	1.487	1.488	1.489	1.486	1.487	1.488	1.488
C_5-N_3	1.380	1.381	1.380	1.381	1.382	1.382	1.383	1.383
C_8-N_3	1.443	1.443	1.443	1.443	1.443	1.443	1.442	1.443
C_4-C_5	1.387	1.386	1.384	1.384	1.387	1.387	1.384	1.384
C_4-C_{20}	1.477	1.478	1.479	1.480	1.480	1.481	1.482	1.482
C_5-C_{15}	1.492	1.492	1.492	1.492	1.493	1.493	1.492	1.493
C_6-S_7	1.847	1.847	1.846	1.846	1.847	1.846	1.846	1.846
C_6-H_{13}	1.089	1.089	1.089	1.088	1.089	1.089	1.089	1.088
C_6-H_{14}	1.092	1.092	1.092	1.092	1.092	1.092	1.092	1.092
C_8-S_7	1.865	1.864	1.863	1.862	1.866	1.865	1.863	1.863
S_7-O_9	1.463	1.463	1.463	1.463	1.463	1.463	1.463	1.463
S_7-O_{10}	1.462	1.462	1.462	1.462	1.462	1.462	1.462	1.462
C_8-H_{11}	1.089	1.090	1.089	1.090	1.089	1.090	1.089	1.090
C_8-H_{12}	1.092	1.091	1.092	1.092	1.092	1.092	1.092	1.092
C_{15}-H_{16}	1.088	1.088	1.088	1.088	1.087	1.087	1.087	1.087
C_{15}-H_{17}	1.095	1.095	1.095	1.095	1.095	1.095	1.095	1.095
C_{15}-H_{18}	1.096	1.095	1.096	1.095	1.096	1.096	1.096	1.096
C_{19}-O_{21}	1.216	1.215	1.206	1.207	1.216	1.216	1.206	1.206
C_{19}-O_{22}	1.343	1.344	1.363	1.362	1.340	1.340	1.362	1.361
C_{20}-O_{23}	1.213	1.213	1.213	1.213	1.207	1.206	1.205	1.205
C_{20}-O_{24}	1.346	1.346	1.343	1.342	1.358	1.358	1.356	1.357
C_{26}-O_{22}	1.439	1.439	1.440	1.440	1.439	1.439	1.440	1.440
C_{25}-O_{24}	1.438	1.438	1.438	1.438	1.440	1.440	1.441	1.441
C_{25}-H_{27}	1.088	1.088	1.088	1.088	1.088	1.088	1.088	1.088
C_{25}-H_{28}	1.091	1.091	1.091	1.091	1.091	1.091	1.090	1.091
C_{25}-H_{29}	1.091	1.091	1.091	1.091	1.091	1.091	1.091	1.090
C_{26}-H_{30}	1.088	1.088	1.088	1.088	1.088	1.088	1.088	1.088
C_{26}-H_{31}	1.091	1.091	1.091	1.091	1.091	1.091	1.091	1.091
C_{26}-H_{32}	1.091	1.091	1.091	1.091	1.091	1.091	1.091	1.091
C_2-C_1-C_4	106.5	106.5	106.6	106.6	106.7	106.7	106.8	106.8
C_2-C_1-C_{19}	120.3	120.5	125.0	125.2	120.9	121.1	125.7	125.9
C_4-C_1-C_{19}	132.8	132.6	127.9	127.6	132.2	132.0	127.1	126.9
C_1-C_2-N_3	108.2	108.2	107.9	107.9	108.1	108.1	107.9	107.9
C_1-C_2-C_6	136.0	136.0	136.7	136.8	136.0	136.0	136.7	136.8

C_6-C_2-N_3	115.7	115.8	115.2	115.3	115.8	115.9	115.3	115.4
C_2-N_3-C_5	110.5	110.6	110.6	110.6	110.6	110.6	110.6	110.6
C_2-N_3-C_8	118.7	119.0	119.0	119.2	118.7	119.0	119.0	119.2
C_5-N_3-C_8	130.6	130.4	130.3	130.2	130.7	130.4	130.4	130.2
C_1-C_4-C_5	108.1	108.1	108.2	108.3	108.0	108.0	108.2	108.2
C_1-C_4-C_{20}	129.5	129.6	128.9	128.8	125.7	125.8	125.2	125.2
C_5-C_4-C_{20}	122.2	122.1	122.7	122.8	125.8	125.6	126.1	126.0
C_4-C_5-N_3	106.7	106.7	106.6	106.6	106.6	106.6	106.5	106.5
C_{15}-C_5-N_3	121.5	121.5	121.7	121.8	120.8	120.8	121.1	121.1
C_4-C_5-C_{15}	131.8	131.8	131.7	131.6	132.6	132.6	132.3	132.3
C_2-C_6-S_7	102.9	103.0	103.3	103.2	102.9	103.1	103.2	103.2
C_2-C_6-H_{13}	113.8	113.4	113.9	113.5	113.8	113.3	113.9	113.5
C_2-C_6-H_{14}	114.0	114.3	114.0	114.4	114.0	114.3	114.0	114.3
S_7-C_6-H_{13}	108.6	108.4	107.9	107.9	108.5	108.4	108.0	108.0
S_7-C_6-H_{14}	107.1	107.0	107.0	106.8	107.1	107.0	107.0	106.7
H_{13}-C_6-H_{14}	109.9	110.2	110.2	110.5	109.9	110.2	110.2	110.4
C_6-S_7-C_8	94.1	94.5	94.2	94.4	94.1	94.6	94.1	94.4
C_6-S_7-O_9	109.4	109.4	109.3	109.3	109.4	109.5	109.3	109.4
C_6-S_7-O_{10}	111.5	111.3	111.3	111.2	111.6	111.2	111.3	111.1
C_8-S_7-O_9	108.1	108.1	108.3	108.3	108.1	108.1	108.2	108.2
C_8-S_7-O_{10}	109.4	109.3	109.5	109.5	109.4	109.2	109.5	109.4
O_9-S_7-O_{10}	121.0	121.0	121.0	120.9	121.0	120.9	120.9	120.9
N_3-C_8-S_7	102.4	102.6	102.5	102.6	102.4	102.7	102.5	102.7
N_3-C_8-H_{11}	112.8	112.9	112.8	112.9	112.9	113.0	112.9	113.0
N_3-C_8-H_{12}	113.4	113.2	113.4	113.3	113.4	113.2	113.5	113.3
S_7-C_8-H_{11}	108.0	107.8	108.0	107.8	107.9	107.7	107.8	107.7
S_7-C_8-H_{12}	107.9	107.9	107.8	107.9	107.8	107.9	107.8	107.8
H_{11}-C_8-H_{12}	111.7	111.7	111.7	111.7	111.7	111.7	111.7	111.6
C_5-C_{15}-H_{16}	109.8	109.7	109.6	109.5	110.1	110.0	109.9	109.9
C_5-C_{15}-H_{17}	111.6	111.1	111.6	111.2	111.5	111.2	111.6	111.3
C_5-C_{15}-H_{18}	111.1	111.6	111.1	111.6	111.2	111.5	111.3	111.6
H_{16}-C_{15}-H_{17}	109.2	107.7	109.1	107.7	108.7	107.7	108.6	107.7
H_{16}-C_{15}-H_{18}	107.3	108.9	107.3	108.8	107.4	108.5	107.4	108.5
H_{17}-C_{15}-H_{18}	107.9	107.8	107.9	107.8	107.8	107.7	107.8	107.8
C_1-C_{19}-O_{21}	123.1	123.3	126.2	126.0	123.1	123.2	125.8	125.7
C_1-C_{19}-O_{22}	113.4	113.4	110.9	111.1	113.1	113.1	111.0	111.2
O_{21}-C_{19}-O_{22}	123.3	123.2	122.9	122.8	123.7	123.6	123.1	123.1
C_4-C_{20}-O_{23}	124.6	124.6	124.5	124.5	125.1	125.1	124.8	124.8
C_4-C_{20}-O_{24}	112.2	112.2	111.9	111.9	112.0	112.0	112.0	112.0
O_{23}-C_{20}-O_{24}	123.1	123.1	123.5	123.6	122.9	122.8	123.2	123.2
C_{19}-O_{22}-C_{26}	115.9	115.9	115.5	115.6	116.2	116.2	115.4	115.5
C_{20}-O_{24}-C_{25}	115.9	115.9	116.1	116.2	115.5	115.5	115.4	115.4
C_{24}-O_{25}-H_{27}	105.4	105.4	105.3	105.3	105.4	105.4	105.4	105.4
C_{24}-O_{25}-H_{28}	110.6	110.4	110.6	110.2	110.3	110.6	110.2	110.6
C_{24}-O_{25}-H_{29}	110.4	110.6	110.2	110.6	110.6	110.4	110.6	110.2
H_{27}-C_{25}-H_{28}	110.6	110.7	110.7	110.5	110.6	110.8	110.7	110.7
H_{27}-C_{25}-H_{29}	110.7	110.6	110.5	110.7	110.7	110.5	110.7	110.7
H_{28}-C_{25}-H_{29}	109.1	109.1	109.4	109.4	109.1	109.1	109.1	109.1
O_{22}-C_{26}-H_{30}	105.4	105.4	105.5	105.5	105.3	105.3	105.5	105.5
O_{22}-C_{26}-H_{31}	110.5	110.4	110.4	110.5	110.5	110.3	110.3	110.5
O_{22}-C_{26}-H_{32}	110.5	110.5	110.6	110.4	110.3	110.5	110.5	110.3
H_{30}-C_{26}-H_{31}	110.6	110.7	110.5	110.7	110.7	110.6	110.6	110.7
H_{30}-C_{26}-H_{32}	110.7	110.6	110.7	110.5	110.6	110.8	110.7	110.6
H_{31}-C_{26}-H_{32}	109.2	109.2	109.1	109.2	109.3	109.3	109.1	109.2

C_4-C_1-C_2-N_3	-0.4	0.3	-0.2	0.1	-0.2	0.1	-0.1	0.0
C_4-C_1-C_2-C_6	-176.3	179.3	-176.7	178.8	-176.9	179.7	-176.6	178.9
C_{19}-C_1-C_2-N_3	173.3	-173.9	172.0	-171.9	175.0	-175.5	172.6	-172.4
C_{19}-C_1-C_2-C_6	-2.7	5.2	-4.4	6.9	-1.7	4.0	-4.0	6.5
C_2-C_1-C_4-C_5	1.0	-0.4	0.8	-0.2	0.6	-0.1	0.5	0.1
C_2-C_1-C_4-C_{20}	-173.4	174.0	-174.9	175.3	-171.7	171.8	-171.8	172.0
C_{19}-C_1-C_4-C_5	-171.6	172.7	-171.1	171.6	-173.8	174.9	-172.0	172.3
C_{19}-C_1-C_4-C_{20}	14.0	-12.8	13.1	-12.9	13.9	-13.2	15.7	-15.8
C_2-C_1-C_{19}-O_{21}	22.4	-20.6	-153.9	154.1	21.3	-19.9	-153.9	154.0
C_2-C_1-C_{19}-O_{22}	-154.2	156.3	23.9	-23.7	-155.9	157.6	24.0	-23.9
C_4-C_1-C_{19}-O_{21}	-165.8	167.1	16.7	-16.1	-164.9	165.7	17.3	-16.9
C_4-C_1-C_{19}-O_{22}	17.5	-16.0	-165.5	166.1	17.9	-16.8	-164.8	165.3
C_1-C_2-N_3-C_5	-0.3	-0.1	-0.4	0.0	-0.3	-0.1	-0.4	-0.1
C_1-C_2-N_3-C_8	-177.3	179.6	-178.1	179.8	-178.0	179.9	-178.3	-179.8
C_6-C_2-N_3-C_5	176.6	-179.3	176.9	-179.0	177.2	-179.8	177.0	-179.2
C_6-C_2-N_3-C_8	-0.5	0.3	-0.8	0.8	-0.6	0.3	-0.9	1.1
C_1-C_2-C_6-S_7	159.5	166.0	160.8	165.2	160.4	165.8	160.9	165.3
C_1-C_2-C_6-H_{13}	42.2	49.1	44.0	48.7	43.2	48.8	44.1	48.7
C_1-C_2-C_6-H_{14}	-84.9	-78.3	-83.5	-79.2	-84.0	-78.5	-83.5	-79.2
N_3-C_2-C_6-S_7	-16.2	-15.0	-15.5	-16.1	-16.1	-14.7	-15.5	-15.9
N_3-C_2-C_6-H_{13}	-133.5	-131.9	-132.2	-132.6	-133.3	-131.7	-132.3	-132.5
N_3-C_2-C_6-H_{14}	99.4	100.7	100.2	99.4	99.5	101.0	100.1	99.6
C_2-N_3-C_5-C_4	0.9	-0.2	0.9	-0.1	0.7	0.1	0.8	0.1
C_2-N_3-C_5-C_{15}	179.1	-178.2	179.4	-178.2	178.4	-177.2	178.6	-177.3
C_8-N_3-C_5-C_4	177.5	-179.7	178.3	-179.9	178.0	-180.0	178.3	179.8
C_8-N_3-C_5-C_{15}	-4.3	2.3	-3.3	2.0	-4.2	2.7	-3.9	2.3
C_2-N_3-C_8-S_7	16.7	14.4	16.4	14.9	16.7	14.2	16.5	14.2
C_2-N_3-C_8-H_{11}	132.5	130.2	132.3	130.7	132.4	129.9	132.3	129.9
C_2-N_3-C_8-H_{12}	-99.3	-101.6	-99.5	-101.2	-99.2	-101.9	-99.4	-101.8
C_5-N_3-C_8-S_7	-159.7	-166.0	-160.7	-165.4	-160.5	-165.8	-160.8	-165.4
C_5-N_3-C_8-H_{11}	-43.8	-50.3	-44.9	-49.6	-44.8	-50.0	-45.0	-49.7
C_5-N_3-C_8-H_{12}	84.4	77.9	83.4	78.6	83.6	78.2	83.3	78.5
C_1-C_4-C_5-N_3	-1.1	0.3	-1.1	0.2	-0.8	0.0	-0.8	-0.1
C_1-C_4-C_5-C_{15}	-179.1	178.0	-179.3	178.1	-178.1	176.8	-178.3	177.0
C_{20}-C_4-C_5-N_3	173.7	-174.6	175.0	-175.7	171.5	-171.9	171.5	-171.9
C_{20}-C_4-C_5-C_{15}	-4.2	3.1	-3.2	2.2	-5.8	4.9	-6.1	5.1
C_1-C_4-C_5-O_{23}	-151.4	148.9	-149.4	147.9	32.9	-34.2	37.6	-38.0
C_1-C_4-C_5-O_{24}	31.5	-34.1	33.2	-34.7	-148.5	147.2	-143.9	143.6
C_5-C_4-C_5-O_{23}	34.9	-37.4	35.4	-37.2	-138.1	136.3	-133.4	132.5
C_5-C_4-C_5-O_{24}	-142.1	139.6	-142.0	140.3	40.5	-42.2	45.1	-46.0
N_3-C_5-C_{15}-H_{16}	-174.3	-179.0	-175.3	-178.5	-173.4	-178.6	-176.4	-177.1
N_3-C_5-C_{15}-H_{17}	-53.2	-60.0	-54.3	-59.6	-52.6	-59.4	-55.7	-58.0
N_3-C_5-C_{15}-H_{18}	67.2	60.3	66.2	60.9	67.7	60.9	64.8	62.5
C_4-C_5-C_{15}-H_{16}	3.4	3.6	2.6	3.9	3.7	4.9	0.9	6.2
C_4-C_5-C_{15}-H_{17}	124.6	122.5	123.6	122.8	124.4	124.2	121.5	125.3
C_4-C_5-C_{15}-H_{18}	-115.1	-117.1	-115.9	-116.7	-115.3	-115.6	-118.0	-114.2
C_2-C_6-S_7-C_8	21.6	19.5	20.9	20.7	21.5	19.1	21.0	20.2
C_2-C_6-S_7-O_9	-89.2	-91.5	-90.1	-90.4	-89.3	-91.9	-89.9	-90.9
C_2-C_6-S_7-O_{10}	134.3	132.3	133.7	133.6	134.2	131.8	133.8	133.0
H_{13}-C_6-S_7-C_8	142.5	139.9	141.8	141.1	142.4	139.4	141.9	140.6
H_{13}-C_6-S_7-O_9	31.7	28.9	30.8	30.0	31.6	28.4	30.9	29.5
H_{13}-C_6-S_7-O_{10}	-104.8	-107.3	-105.4	-106.0	-104.9	-107.9	-105.3	-106.6
H_{14}-C_6-S_7-C_8	-98.9	-101.3	-99.7	-100.2	-99.0	-101.7	-99.6	-100.6
H_{14}-C_6-S_7-O_9	150.3	147.8	149.3	148.8	150.3	147.2	149.5	148.2

H_{14}-C_6-S_7-O_{10}	13.9	11.5	13.1	12.7	13.8	10.9	13.3	12.2
C_6-S_7-C_8-N_3	-21.8	-19.4	-21.2	-20.3	-21.7	-19.0	-21.3	-19.6
C_6-S_7-C_8-H_{11}	-141.0	-138.8	-140.5	-139.7	-141.0	-138.5	-140.6	-139.1
C_6-S_7-C_8-H_{12}	98.1	100.4	98.7	99.6	98.2	100.9	98.7	100.3
O_9-S_7-C_8-N_3	90.1	92.8	90.7	91.7	90.2	93.3	90.6	92.5
O_9-S_7-C_8-H_{11}	-29.2	-26.7	-28.6	-27.7	-29.1	-26.2	-28.7	-27.0
O_9-S_7-C_8-H_{12}	-150.0	-147.4	-149.4	-148.5	-149.9	-146.9	-149.4	-147.6
O_{10}-S_7-C_8-N_3	-136.3	-133.8	-135.5	-134.6	-136.3	-133.4	-135.7	-133.9
O_{10}-S_7-C_8-H_{11}	104.4	106.8	105.2	106.0	104.4	107.2	105.0	106.7
O_{10}-S_7-C_8-H_{12}	-16.4	-14.0	-15.6	-14.8	-16.4	-13.5	-15.7	-13.9
C_1-C_{19}-O_{22}-C_{26}	178.9	-179.4	-177.2	177.5	-178.4	178.0	-177.9	178.3
O_{21}-C_{19}-O_{22}-C_{26}	2.3	-2.5	0.8	-0.3	4.4	-4.6	0.1	0.3
C_4-C_{20}-O_{24}-C_{25}	-178.6	178.7	-175.8	175.9	-178.1	177.7	-179.2	178.8
O_{23}-C_{20}-O_{24}-C_{25}	4.3	-4.2	6.7	-6.6	0.5	-0.9	-0.8	0.3
C_{19}-O_{22}-C_{26}-H_{30}	179.4	-179.7	179.4	-179.4	177.9	-178.3	-179.8	-179.6
C_{19}-O_{22}-C_{26}-H_{31}	-61.2	-60.2	-61.2	-59.7	-62.5	-59.1	-60.4	-59.9
C_{19}-O_{22}-C_{26}-H_{32}	59.8	60.8	59.7	61.2	58.5	62.0	60.5	60.9
C_{20}-O_{24}-C_{25}-H_{27}	178.7	-178.6	177.8	-178.5	179.7	-178.9	-179.4	179.5
C_{20}-O_{24}-C_{25}-H_{28}	-61.8	-59.0	-62.5	-59.3	-60.9	-59.1	-59.9	-60.8
C_{20}-O_{24}-C_{25}-H_{29}	59.2	61.9	58.6	61.8	59.9	61.7	60.9	60.0

Table 2S. Definition of internal coordinates used in the normal mode analysis of PTD.

Definition[a]	Vibration
ν_1	$\nu(C_1\text{-}C_2)$
ν_2	$\nu(C_1\text{-}C_4)$
ν_3	$\nu(C_1\text{-}C_{19})$
ν_4	$\nu(C_2\text{-}N_3)$
ν_5	$\nu(C_2\text{-}C_6)$
ν_6	$\nu(C_5\text{-}N_3)$
ν_7	$\nu(C_8\text{-}N_3)$
ν_8	$\nu(C_4\text{-}C_5)$
ν_9	$\nu(C_4\text{-}C_{20})$
ν_{10}	$\nu(C_5\text{-}C_{15})$
ν_{11}	$\nu(C_6\text{-}S_7)$
ν_{12}	$\nu(C_6\text{-}H_{13})$
ν_{13}	$\nu(C_6\text{-}H_{14})$
ν_{14}	$\nu(C_8\text{-}S_7)$
ν_{15}	$\nu(S_7\text{-}O_9)$
ν_{16}	$\nu(S_7\text{-}O_{10})$
ν_{17}	$\nu(C_8\text{-}H_{11})$
ν_{18}	$\nu(C_8\text{-}H_{12})$
ν_{19}	$\nu(C_{15}\text{-}H_{16})$
ν_{20}	$\nu(C_{15}\text{-}H_{17})$
ν_{21}	$\nu(C_{15}\text{-}H_{18})$
ν_{22}	$\nu(C_{19}\text{-}O_{21})$
ν_{23}	$\nu(C_{19}\text{-}O_{22})$
ν_{24}	$\nu(C_{20}\text{-}O_{23})$
ν_{25}	$\nu(C_{20}\text{-}O_{24})$
ν_{26}	$\nu(C_{26}\text{-}O_{22})$
ν_{27}	$\nu(C_{25}\text{-}O_{24})$
ν_{28}	$\nu(C_{25}\text{-}H_{27})$
ν_{29}	$\nu(C_{25}\text{-}H_{28})$
ν_{30}	$\nu(C_{25}\text{-}H_{29})$
ν_{31}	$\nu(C_{26}\text{-}H_{30})$
ν_{32}	$\nu(C_{26}\text{-}H_{31})$
ν_{33}	$\nu(C_{26}\text{-}H_{32})$

δ_1	$\delta(C_2\text{-}C_1\text{-}C_4) - 0.8\ \delta(N_3\text{-}C_2\text{-}C_1) - 0.8\ \delta(C_1\text{-}C_4\text{-}C_5) + 0.3\ \delta(C_5\text{-}N_3\text{-}C_2) + 0.3\ \delta(C_4\text{-}C_5\text{-}N_3)$
δ_2	$-1.1\ \delta(N_3\text{-}C_2\text{-}C_1) + 1.1\ \delta(C_1\text{-}C_4\text{-}C_5) + 1.8\ \delta(C_5\text{-}N_3\text{-}C_2) - 1.8\ \delta(C_4\text{-}C_5\text{-}N_3)$
δ_3	$\delta(C_6\text{-}C_2\text{-}N_3) - 0.8\ \delta(C_2\text{-}N_3\text{-}C_8) - 0.8\ \delta(S_7\text{-}C_6\text{-}C_2) + 0.3\ \delta(N_3\text{-}C_8\text{-}S_7) + 0.3\ \delta(C_8\text{-}S_7\text{-}C_6)$
δ_4	$-1.1\ \delta(C_2\text{-}N_3\text{-}C_8) + 1.1\ \delta(S_7\text{-}C_6\text{-}C_2) + 1.8\ \delta(N_3\text{-}S_7\text{-}C_8) - 1.8\ \delta(C_8\text{-}S_7\text{-}C_6)$
δ_5	$\delta(C_6\text{-}S_7\text{-}O_9) - \delta(C_8\text{-}S_7\text{-}O_9)$
δ_6	$\delta(C_6\text{-}S_7\text{-}O_{10}) - \delta(C_8\text{-}S_7\text{-}O_{10})$
δ_7	$\delta(C_2\text{-}C_1\text{-}C_{19}) - \delta(C_4\text{-}C_1\text{-}C_{19})$
δ_8	$\delta(C_1\text{-}C_4\text{-}C_{20}) - \delta(C_5\text{-}C_4\text{-}C_{20})$
δ_9	$\delta(C_4\text{-}C_5\text{-}C_{15}) - \delta(N_3\text{-}C_5\text{-}C_{15})$
δ_{10}	$\delta(N_3\text{-}C_8\text{-}H_{11}) - \delta(S_7\text{-}C_8\text{-}H_{11})$
δ_{11}	$\delta(N_3\text{-}C_8\text{-}H_{12}) - \delta(S_7\text{-}C_8\text{-}H_{12})$
δ_{12}	$\delta(C_2\text{-}C_6\text{-}H_{13}) - \delta(S_7\text{-}C_6\text{-}H_{13})$
δ_{13}	$\delta(C_2\text{-}C_6\text{-}H_{14}) - \delta(S_7\text{-}C_6\text{-}H_{14})$
δ_{14}	$\delta(H_{16}\text{-}C_{15}\text{-}H_{17}) + \delta(H_{16}\text{-}C_{15}\text{-}H_{18}) + \delta(H_{17}\text{-}C_{15}\text{-}H_{18}) - \delta(C_5\text{-}C_{15}\text{-}H_{16}) - \delta(C_5\text{-}C_{15}\text{-}H_{17}) - \delta(C_5\text{-}C_{15}\text{-}H_{18})$
δ_{15}	$2\ \delta(H_{16}\text{-}C_{15}\text{-}H_{17}) - \delta(H_{16}\text{-}C_{15}\text{-}H_{18}) - \delta(H_{17}\text{-}C_{15}\text{-}H_{18})$
δ_{16}	$\delta(C_5\text{-}C_{15}\text{-}H_{16}) - \delta(C_5\text{-}C_{15}\text{-}H_{17})$
δ_{17}	$2\ \delta(C_5\text{-}C_{15}\text{-}H_{16}) - \delta(C_5\text{-}C_{15}\text{-}H_{17}) - \delta(C_5\text{-}C_{15}\text{-}H_{18})$
δ_{18}	$\delta(C_5\text{-}C_{15}\text{-}H_{17}) - \delta(C_5\text{-}C_{15}\text{-}H_{18})$
δ_{19}	$\delta(H_{27}\text{-}C_{25}\text{-}H_{28}) + \delta(H_{27}\text{-}C_{25}\text{-}H_{29}) + \delta(H_{28}\text{-}C_{25}\text{-}H_{29}) - \delta(O_{24}\text{-}C_{25}\text{-}H_{27}) - \delta(O_{24}\text{-}C_{25}\text{-}H_{28}) - \delta(O_{24}\text{-}C_{25}\text{-}H_{29})$
δ_{20}	$2\ \delta(H_{27}\text{-}C_{25}\text{-}H_{28}) - \delta(H_{27}\text{-}C_{25}\text{-}H_{29}) - \delta(H_{28}\text{-}C_{25}\text{-}H_{29})$
δ_{21}	$\delta(H_{27}\text{-}C_{25}\text{-}H_{29}) - \delta(H_{28}\text{-}C_{25}\text{-}H_{29})$
δ_{22}	$2\ \delta(O_{24}\text{-}C_{25}\text{-}H_{27}) - \delta(O_{24}\text{-}C_{25}\text{-}H_{28}) - \delta(O_{24}\text{-}C_{25}\text{-}H_{29})$
δ_{23}	$\delta(O_{24}\text{-}C_{25}\text{-}H_{28}) - \delta(O_{24}\text{-}C_{25}\text{-}H_{29})$
δ_{24}	$\delta(H_{30}\text{-}C_{26}\text{-}H_{31}) + \delta(H_{30}\text{-}C_{26}\text{-}H_{32}) + \delta(H_{31}\text{-}C_{26}\text{-}H_{32}) - \delta(O_{22}\text{-}C_{26}\text{-}H_{30}) - \delta(O_{22}\text{-}C_{26}\text{-}H_{31}) - \delta(O_{22}\text{-}C_{26}\text{-}H_{32})$
δ_{25}	$2\ \delta(H_{30}\text{-}C_{26}\text{-}H_{31}) - \delta(H_{30}\text{-}C_{26}\text{-}H_{32}) - \delta(H_{31}\text{-}C_{26}\text{-}H_{32})$
δ_{26}	$\delta(H_{30}\text{-}C_{26}\text{-}H_{32}) - \delta(H_{31}\text{-}C_{26}\text{-}H_{32})$
δ_{27}	$2\ \delta(O_{22}\text{-}C_{26}\text{-}H_{30}) - \delta(O_{22}\text{-}C_{26}\text{-}H_{31}) - \delta(O_{22}\text{-}C_{26}\text{-}H_{32})$
δ_{28}	$\delta(O_{22}\text{-}C_{26}\text{-}H_{31}) - \delta(O_{22}\text{-}C_{26}\text{-}H_{32})$
δ_{29}	$2\ \delta(C_1\text{-}C_{19}\text{-}O_{21}) - \delta(O_{21}\text{-}C_{19}\text{-}O_{22}) - \delta(C_1\text{-}C_{19}\text{-}O_{22})$
δ_{30}	$\delta(O_{21}\text{-}C_{19}\text{-}O_{22}) - \delta(C_1\text{-}C_{19}\text{-}O_{22})$
δ_{31}	$2\ \delta(C_4\text{-}C_{20}\text{-}O_{23}) - \delta(O_{23}\text{-}C_{20}\text{-}O_{24}) - \delta(C_4\text{-}C_{20}\text{-}O_{24})$
δ_{32}	$\delta(O_{23}\text{-}C_{20}\text{-}O_{24}) - \delta(C_4\text{-}C_{20}\text{-}O_{24})$
δ_{33}	$\delta(C_{19}\text{-}O_{22}\text{-}C_{26})$
δ_{34}	$\delta(C_{20}\text{-}O_{24}\text{-}C_{25})$
γ_1	$\gamma\ (C_6\text{-}S_7(\text{-}O_9)\text{-}C_8)$

γ_2	$\gamma\,(C_6\text{-}S_7(\text{-}O_{10})\text{-}C_8)$
γ_3	$\gamma\,(C_2\text{-}C_1(\text{-}O_{19})\text{-}C_4)$
γ_4	$\gamma\,(C_1\text{-}C_4(\text{-}O_{20})\text{-}C_5)$
γ_5	$\gamma\,(C_4\text{-}C_5(\text{-}C_{15})\text{-}N_3)$
γ_6	$\gamma\,(N_3\text{-}C_8(\text{-}H_{11})\text{-}S_7)$
γ_7	$\gamma\,(N_3\text{-}C_8(\text{-}H_{12})\text{-}S_7)$
γ_8	$\gamma\,(C_2\text{-}C_6(\text{-}H_{13})\text{-}S_7)$
γ_9	$\gamma\,(C_2\text{-}C_6(\text{-}H_{14})\text{-}S_7)$
γ_{10}	$\gamma\,(C_1\text{-}C_{19}(\text{-}O_{21})\text{-}O_{22})$
γ_{11}	$\gamma\,(C_4\text{-}C_{20}(\text{-}O_{23})\text{-}O_{24})$
τ_1	$0.3\ \delta(C_4\text{-}C_1\text{-}C_2\text{-}N_3) + 0.3\ \delta(C_5\text{-}C_4\text{-}C_1\text{-}C_2) - 0.8\ \delta(C_5\text{-}N_3\text{-}C_2\text{-}C_1) - 0.8\ \delta(C_1\text{-}C_4\text{-}C_5\text{-}N_3) + \delta(C_4\text{-}C_5\text{-}N_3\text{-}C_2)$
τ_2	$-1.1\ \delta(C_1\text{-}C_4\text{-}C_5\text{-}N_3) + 1.1\ \delta(C_5\text{-}N_3\text{-}C_2\text{-}C_1) + 1.8\ \delta(C_5\text{-}C_4\text{-}C_1\text{-}C_2) - 1.8\ \delta(C_4\text{-}C_1\text{-}C_2\text{-}N_3)$
τ_3	$0.3\ \delta(C_6\text{-}C_2\text{-}N_3\text{-}C_8) + 0.3\ \delta(S_7\text{-}C_6\text{-}C_2\text{-}N_3) - 0.8\ \delta(C_2\text{-}N_3\text{-}C_8\text{-}S_7) - 0.8\ \delta(C_8\text{-}S_7\text{-}C_6\text{-}C_2) + \delta(N_3\text{-}S_7\text{-}S_7\text{-}C_6)$
τ_4	$-1.1\ \delta(C_8\text{-}S_7\text{-}C_6\text{-}C_2) + 1.1\ \delta(C_2\text{-}N_3\text{-}C_8\text{-}S_7) + 1.8\ \delta(S_7\text{-}C_6\text{-}C_2\text{-}N_3) - 1.8\ \delta(C_6\text{-}C_2\text{-}N_3\text{-}C_8)$
τ_5	$\delta(C_1\text{-}C_2\text{-}N_3\text{-}C_8) - \delta(C_6\text{-}C_2\text{-}N_3\text{-}C_5)$
τ_6	$\delta(C_2\text{-}C_1\text{-}C_{19}\text{-}O_{21}) + \delta(C_4\text{-}C_1\text{-}C_{19}\text{-}O_{21}) + \delta(C_2\text{-}C_1\text{-}C_{19}\text{-}O_{22}) + \delta(C_2\text{-}C_1\text{-}C_{19}\text{-}O_{22})$
τ_7	$\delta(C_1\text{-}C_4\text{-}C_{20}\text{-}O_{23}) + \delta(C_1\text{-}C_4\text{-}C_{20}\text{-}O_{23}) + \delta(C_1\text{-}C_4\text{-}C_{20}\text{-}O_{24}) + \delta(C_1\text{-}C_4\text{-}C_{20}\text{-}O_{24})$
τ_8	$\delta(N_3\text{-}C_5\text{-}C_{15}\text{-}H_{16}) + \delta(C_4\text{-}C_5\text{-}C_{15}\text{-}H_{16}) + \delta(N_3\text{-}C_5\text{-}C_{15}\text{-}H_{17}) + \delta(C_4\text{-}C_5\text{-}C_{15}\text{-}H_{17}) + \delta(N_3\text{-}C_5\text{-}C_{15}\text{-}H_{18}) + \delta(C_4\text{-}C_5\text{-}C_{15}\text{-}H_{18})$
τ_9	$\delta(C_1\text{-}C_{19}\text{-}O_{22}\text{-}C_{26}) + \delta(O_{21}\text{-}C_{19}\text{-}O_{22}\text{-}C_{26})$
τ_{10}	$\delta(C_4\text{-}C_{20}\text{-}O_{24}\text{-}C_{25}) + \delta(O_{23}\text{-}C_{20}\text{-}O_{24}\text{-}C_{25})$
τ_{11}	$\delta(C_{19}\text{-}O_{22}\text{-}C_{26}\text{-}H_{30}) + \delta(C_{19}\text{-}O_{22}\text{-}C_{26}\text{-}H_{31}) + \delta(C_{19}\text{-}O_{22}\text{-}C_{26}\text{-}H_{32})$
τ_{12}	$\delta(C_{20}\text{-}O_{24}\text{-}C_{25}\text{-}H_{27}) + \delta(C_{20}\text{-}O_{24}\text{-}C_{25}\text{-}H_{28}) + \delta(C_{20}\text{-}O_{24}\text{-}C_{25}\text{-}H_{29})$

[a] ν, δ, γ, and τ denote stretching, in-plane bending, out-of plane bending, and torsion vibrations, respectively.

Table 3S. Assignment of experimental spectra of PTD in Ar and Xe matrices at 11 and 20 K, respectively. Harmonic frequencies (in cm^{-1}) and integral intensities (in km/mol) are calculated at B3LYP/6-311++G(d,p) level. Relative experimental (in % relative to the 1146 and 1145 cm^{-1} in Ar and Xe, respectively) and calculated integral intensities (in km mol^{-1}) scaled by the abundance of the conformers at 423 K are given in parenthesis.

$\nu_{exp,\ Ar}$ (cm^{-1})	$\nu_{exp,\ Xe}$ (cm^{-1})	$\nu_{calc\ 423K}$ (cm^{-1})[c]	Conformer	Assignment[e]
3030[a] (9.3)	3021(9.6)	3128 (1)	**V**	ν_{31}(81), ν_{33}(11)
		3128 (1)	**VI**	ν_{31}(81), ν_{32}(11)
		3127 (2)	**III**	ν_{28}(81), ν_{30}(11)
		3127 (1)	**IV**	ν_{28}(81), ν_{29}(11)
		3125 (4)	**I**	ν_{31}(80), ν_{33}(10)
		3125 (3)	**II**	ν_{31}(80), ν_{32}(10)
		3124 (3)	**II**	ν_{28}(80), ν_{29}(10)
		3123 (4)	**I**	ν_{28}(80), ν_{30}(10)
		3123 (1)	**IV**	ν_{31}(79), ν_{33}(11), ν_{32}(10)
		3123 (1)	**V**	ν_{28}(79), ν_{29}(12)
		3122 (2)	**III**	ν_{31}(79), ν_{32}(11), ν_{33}(10)
		3122 (1)	**VI**	ν_{28}(79), ν_{30}(11)
		3116 (1)	**II**	ν_{12}(81), ν_{13}(17)
		3110 (1)	**I**	ν_{12}(73), ν_{13}(21)
3003 (13.1)	2992 (11.9)	3093 (2)	**III**	ν_{32}(51), ν_{33}(49)
		3093 (2)	**IV**	ν_{33}(51), ν_{32}(48)
		3093 (2)	**IV**	ν_{29}(51), ν_{30}(49)
		3093 (2)	**V**	ν_{33}(51), ν_{32}(48)
		3093 (1)	**VI**	ν_{32}(51), ν_{33}(48)
		3092 (5)	**I**	ν_{32}(50), ν_{33}(49)
		3092 (4)	**II**	ν_{33}(50), ν_{32}(49)
		3092 (2)	**III**	ν_{30}(51), ν_{29}(49)
		3092 (2)	**V**	ν_{29}(52), ν_{30}(48)
		3092 (1)	**VI**	ν_{30}(51), ν_{29}(48)
		3090 (6)	**I**	ν_{29}(51), ν_{30}(49)
		3090 (5)	**II**	ν_{30}(51), ν_{29}(49)
2959 (23.4)	2947 (29.6)	3044 (1)	**I**	ν_{13}(78), ν_{12}(21)
		3042 (1)	**III**	ν_{12}(80), ν_{13}(29)

		3041 (1)	**II**	ν_{13}(81), ν_{12}(17)
		3038 (1)	**IV**	ν_{13}(82), ν_{12}(15)
		3037 (4)	**I**	ν_{18}(72), ν_{17}(25)
		3037 (3)	**II**	ν_{18}(69), ν_{17}(29)
		3036 (2)	**III**	ν_{18}(71), ν_{17}(25)
		3036 (1)	**VI**	ν_{18}(69), ν_{17}(29)
		3035 (1)	**IV**	ν_{18}(68), ν_{17}(28)
		3035 (1)	**V**	ν_{18}(71), ν_{17}(25)
		3033 (3)	**I**	ν_{20}(51), ν_{21}(46)
		3033 (2)	**III**	ν_{20}(49), ν_{21}(48)
		3032 (3)	**II**	ν_{20}(55), ν_{21}(44)
		3032 (1)	**IV**	ν_{20}(56), ν_{21}(43)
		3032 (1)	**V**	ν_{20}(55), ν_{21}(42)
		3031 (1)	**VI**	ν_{20}(54), ν_{21}(46)
		3021 (11)	**II**	ν_{33}(39), ν_{32}(39), ν_{31}(19)
		3021 (5)	**IV**	ν_{32}(27), ν_{33}(24), ν_{30}(16), ν_{29}(14), ν_{31}(13)
		3021 (4)	**V**	ν_{32}(44), ν_{33}(37), ν_{31}(18)
		3021 (3)	**VI**	ν_{33}(44), ν_{32}(37), ν_{31}(18)
		3020 (13)	**I**	ν_{33}(40), ν_{32}(39), ν_{31}(18)
		3020 (6)	**III**	ν_{29}(38), ν_{30}(32), ν_{28}(16)
		3020 (5)	**III**	ν_{33}(35), ν_{32}(33), ν_{31}(17)
		3020 (4)	**IV**	ν_{28}(28), ν_{29}(24), ν_{32}(15), ν_{33}(13), ν_{28}(12)
		3020 (4)	**V**	ν_{30}(43), ν_{29}(39), ν_{28}(20)
		3020 (3)	**VI**	ν_{29}(42), ν_{30}(37), ν_{28}(20)
		3019 (10)	**I**	ν_{30}(39), ν_{29}(39), ν_{28}(18)
		3019 (9)	**II**	ν_{29}(40), ν_{30}(39), ν_{28}(19)
2910[a]		2989 (7)	**I**	ν_{21}(50), ν_{20}(43)
		2989 (4)	**III**	ν_{21}(48), ν_{20}(44)
		2989 (2)	**V**	ν_{21}(55), ν_{20}(39)
		2989 (2)	**VI**	ν_{21}(51), ν_{20}(43)
		2988 (7)	**II**	ν_{21}(52), ν_{20}(41)
		2988 (3)	**IV**	ν_{21}(53), ν_{20}(40)
1751 (89.8)	1746 (64.8)	1766 (58)	**III**	ν_{22}(77)

		1764 (42)	**IV**	ν_{22}(77)
		1763 (23)	**VI**	ν_{24}(79)
		1761 (32)	**V**	ν_{24}(78)
1720[a,b]	1719[a]	1735 (34)	**IV**	ν_{24}(77)
		1734 (45)	**III**	ν_{24}(77)
		1734 (59)	**I**	ν_{24}(73)
		1734 (50)	**II**	ν_{24}(73)
1713 (143.1), 1709[a,b]	1711[a], 1706[a,b], 1703 (83.6)	1721 (102)	**II**	ν_{22}(72)
		1720 (115)	**I**	ν_{22}(73)
		1723 (19)	**VI**	ν_{22}(76)
		1721 (26)	**V**	ν_{22}(76)
	1695[a,b]			
1590 (14.2)	1586[a]	1592 (6)	**V**	ν_1(52), ν_5(11)
		1591 (4)	**VI**	ν_1(50), ν_5(11), ν_8(10)
		1586 (15)	**I**	ν_1(47), ν_8(12), ν_5(11)
		1586 (12)	**II**	ν_1(45), ν_8(14), ν_5(10)
		1585 (2)	**III**	ν_1(35), ν_8(26)
		1585 (1)	**IV**	ν_1(33), ν_8(28)
1549 (46.6)	1550 (42.2)	1552 (18)	**III**	ν_1(52), ν_5(11)
		1552 (13)	**IV**	ν_8(27), ν_1(26)
		1551 (49)	**I**	ν_8(40), ν_1(12), ν_{10}(10)
		1551 (43)	**II**	ν_8(38), ν_1(15), ν_{10}(10)
	1547[a,b]	1548 (6)	**VI**	ν_8(42), ν_{10}(11), ν_1(10)
		1547 (7)	**V**	ν_8(44), ν_{10}(12)
1463[b] (9.0)	1456[a,b]	1485 (1)	**IV**	δ_{26}(65), δ_{25}(15), δ_{27}(11)
		1484 (1)	**III**	δ_{26}(56), δ_{25}(24), δ_{27}(11)
		1483 (4)	**I**	δ_{21}(35), δ_{20}(18), δ_{26}(12)
		1483 (2)	**II**	δ_{26}(50), δ_{21}(15), δ_{25}(13)
		1482 (1)	**I**	δ_{26}(41), δ_{25}(16), δ_{16}(10)
		1482 (4)	**I**	δ_{16}(43), δ_{15}(13), δ_{21}(12)
		1482 (1)	**II**	δ_{15}(58), γ_6(14), γ_7(13)
		1482 (3)	**II**	δ_{21}(49), δ_{20}(12), δ_{26}(11)
		1482 (2)	**III**	δ_{16}(49), δ_{15}(16), δ_{17}(10)

		1482 (1)	**IV**	$\delta_{15}(67)$, $\gamma_{6}(11)$, $\gamma_{7}(10)$
		1481 (1)	**III**	$\delta_{21}(48)$, $\delta_{20}(20)$, $\delta_{16}(10)$, $\delta_{22}(10)$
		1481 (1)	**IV**	$\delta_{21}(61)$, $\delta_{20}(18)$, $\delta_{22}(11)$
		1481 (1)	**V**	$\delta_{21}(56)$, $\delta_{25}(22)$, $\delta_{27}(11)$
		1481 (1)	**VI**	$\delta_{26}(59)$, $\delta_{25}(18)$, $\delta_{27}(11)$
		1480 (1)	**V**	$\delta_{16}(48)$, $\delta_{15}(20)$
		1476 (1)	**I**	$\gamma_{6}(34)$, $\gamma_{7}(32)$, $\delta_{16}(12)$
		1476 (3)	**II**	$\delta_{15}(39)$, $\gamma_{7}(19)$, $\gamma_{6}(18)$
		1476 (1)	**IV**	$\delta_{15}(31)$, $\gamma_{7}(23)$, $\gamma_{6}(22)$
		1475 (1)	**VI**	$\delta_{15}(46)$, $\gamma_{6}(12)$, $\delta_{16}(12)$, $\gamma_{7}(12)$
1450[a]	1447 (91)	1469 (1)	**IV**	$\delta_{20}(64)$, $\delta_{21}(16)$
		1469 (1)	**VI**	$\delta_{16}(51)$
		1468 (2)	**III**	$\delta_{20}(64)$, $\delta_{21}(27)$
		1468 (1)	**IV**	$\delta_{16}(50)$, $\delta_{25}(13)$
		1468 (1)	**IV**	$\delta_{25}(57)$, $\delta_{26}(15)$, $\delta_{16}(12)$
		1468 (1)	**V**	$\delta_{25}(66)$, $\delta_{26}(26)$
		1468 (1)	**VI**	$\delta_{25}(70)$, $\delta_{26}(19)$
		1467 (5)	**I**	$\delta_{20}(34)$, $\delta_{25}(28)$, $\delta_{21}(17)$, $\delta_{26}(12)$
		1467 (5)	**II**	$\delta_{16}(64)$
		1467 (3)	**II**	$\delta_{25}(39)$, $\delta_{20}(30)$, $\delta_{26}(11)$
		1467 (1)	**III**	$\delta_{25}(65)$, $\delta_{26}(24)$
		1467 (2)	**V**	$\delta_{20}(55)$, $\delta_{21}(17)$, $\delta_{15}(10)$
		1467 (1)	**VI**	$\delta_{20}(67)$, $\delta_{21}(16)$
		1466 (1)	**V**	$\delta_{15}(42)$, $\delta_{21}(10)$
		1463 (2)	**III**	$\delta_{15}(63)$
		1462 (5)	**I**	$\delta_{15}(64)$
		1460 (21)	**I**	$\delta_{24}(47)$, $\delta_{19}(18)$
		1460 (5)	**IV**	$\delta_{24}(37)$, $\delta_{19}(26)$
		1460 (3)	**VI**	$\delta_{24}(63)$
		1459 (18)	**II**	$\delta_{24}(45)$, $\delta_{19}(22)$
		1459 (8)	**III**	$\delta_{19}(37)$, $\delta_{24}(27)$
		1459 (5)	**V**	$\delta_{24}(60)$
1440 (15.9)	1437 (13.1)	1456 (2)	**IV**	$\delta_{19}(46)$, $\delta_{24}(35)$

		1455 (4)	**I**	$\delta_{19}(54)$, $\delta_{24}(26)$
		1455 (4)	**II**	$\delta_{19}(53)$, $\delta_{24}(29)$
		1455 (2)	**III**	$\delta_{24}(45)$, $\delta_{19}(36)$
		1455 (3)	**V**	$\delta_{19}(66)$, $\delta_{24}(11)$
		1455 (2)	**VI**	$\delta_{19}(68)$, $\delta_{24}(10)$
1419 (27.2)	1417 (22.8)	1443 (1)	**II**	$\gamma_{8}(43)$, $\gamma_{9}(39)$
		1443 (1)	**VI**	$\gamma_{8}(41)$, $\gamma_{9}(38)$
		1440 (1)	**III**	$\gamma_{9}(41)$, $\gamma_{8}(40)$
		1439 (2)	**I**	$\gamma_{8}(40)$, $\gamma_{9}(40)$
		1437 (1)	**V**	$\gamma_{9}(36)$, $\gamma_{8}(36)$
		1429 (16)	**III**	$\nu_{2}(23)$
		1429 (12)	**IV**	$\nu_{2}(24)$
		1427 (14)	**V**	$\nu_{2}(22)$
		1426 (10)	**VI**	$\nu_{2}(22)$
		1424 (45)	**I**	$\nu_{2}(20)$, $\nu_{6}(11)$
		1424 (37)	**II**	$\nu_{2}(19)$, $\nu_{6}(11)$, $\nu_{4}(10)$
1409 (5.8)	1405[a]	1409 (1)	**V**	$\delta_{14}(74)$
		1408 (1)	**VI**	$\delta_{14}(67)$
		1405 (2)	**III**	$\delta_{14}(87)$
		1404 (5)	**I**	$\delta_{14}(85)$
		1404 (2)	**IV**	$\delta_{14}(87)$
		1403 (4)	**II**	$\delta_{14}(85)$
1397 (9.7)	1398[a]	1399 (12)	**II**	$\nu_{4}(23)$, $\delta_{2}(13)$, $\nu_{2}(13)$, $\nu_{7}(12)$
		1398 (2)	**VI**	$\nu_{4}(26)$, $\delta_{14}(17)$, $\nu_{7}(10)$
		1397 (10)	**I**	$\nu_{4}(20)$, $\nu_{7}(15)$, $\delta_{2}(13)$, $\nu_{2}(12)$
		1396 (3)	**V**	$\nu_{4}(27)$, $\nu_{7}(14)$, $\delta_{14}(12)$, $\delta_{2}(10)$
		1395 (1)	**IV**	$\nu_{4}(23)$, $\nu_{7}(19)$, $\delta_{2}(12)$
		1394 (3)	**III**	$\nu_{7}(21)$, $\nu_{4}(18)$, $\delta_{2}(12)$
		1385 (10)	**I**	$\nu_{6}(27)$, $\delta_{1}(19)$, $\nu_{4}(14)$
1392[a]		1384 (9)	**III**	$\nu_{6}(25)$, $\delta_{1}(19)$, $\nu_{4}(18)$
		1384 (2)	**V**	$\nu_{6}(30)$, $\delta_{1}(19)$
1382 (2.5)		1383 (8)	**II**	$\nu_{6}(30)$, $\delta_{1}(18)$
		1383 (7)	**IV**	$\nu_{6}(28)$, $\delta_{1}(19)$

		1382 (2)	**VI**	$\nu_6(32)$, $\delta_1(18)$
1367 (61.8)	1362 (68.7)	1352 (61)[d]	**I**	$\nu_{16}(44)$, $\nu_{15}(38)$
1357[a]	1351	1352 (55)[d]	**II**	$\nu_{16}(43)$, $\nu_{15}(39)$
1349 (3.7)	1344 (3.5)	1352 (31)[d]	**III**	$\nu_{16}(43)$, $\nu_{15}(39)$
		1352 (17)[d]	**IV**	$\nu_{16}(44)$, $\nu_{15}(38)$
		1351 (20)[d]	**V**	$\nu_{16}(42)$, $\nu_{15}(39)$
		1351 (14)[d]	**VI**	$\nu_{16}(43)$, $\nu_{15}(39)$
1330 (3.7) *?*				
1315[a]	1315 (13.3)	1311 (23)	**V**	$\nu_{23}(17)$, $\nu_3(17)$, $\nu_9(11)$
		1310 (16)	**VI**	$\nu_{23}(17)$, $\nu_3(17)$, $\nu_9(11)$
1304 (89.4)	1304 (35.4)	1307 (31)	**I**	$\nu_3(15)$, $\nu_{23}(13)$, $\nu_9(12)$
		1306 (20)	**II**	$\nu_3(15)$, $\nu_9(12)$, $\nu_{23}(12)$
		1298 (28)	**III**	$\nu_{25}(16)$, $\nu_9(16)$, $\nu_3(12)$
		1298 (26)	**IV**	$\nu_{25}(16)$, $\nu_9(15)$, $\nu_3(11)$
1247 (62.5)	1249[b] (29.5), 1242[a]	1247 (87)	**I**	$\delta_{11}(23)$, $\delta_{10}(15)$, $\nu_{23}(13)$
		1247 (67)	**II**	$\delta_{11}(25)$, $\delta_{10}(16)$, $\nu_{23}(12)$
		1246 (7)	**VI**	$\delta_{11}(30)$, $\delta_{10}(22)$
		1244 (7)	**V**	$\delta_{11}(30)$, $\delta_{10}(21)$
		1242 (5)	**III**	$\delta_{11}(32)$, $\delta_{10}(21)$, $\nu_7(11)$
		1241 (5)	**IV**	$\delta_{11}(31)$, $\delta_{10}(21)$, $\nu_7(11)$
1237[a]	1233[a,b]	1235 (140)	**II**	$\nu_{25}(23)$
		1234 (147)	**I**	$\nu_{25}(21)$, $\delta_{11}(10)$
1216[a]	1216[a]	1218 (13)	**IV**	$\delta_{13}(19)$, $\delta_{12}(14)$, $\nu_{25}(12)$, $\nu_5(10)$
		1217 (14)	**III**	$\delta_{13}(18)$, $\delta_{12}(14)$, $\nu_{25}(12)$, $\nu_5(10)$
1223[a,b]		1216 (13)	**V**	$\delta_{13}(14)$, $\delta_{12}(11)$, $\nu_{25}(10)$
		1216 (6)	**VI**	$\delta_{13}(15)$, $\delta_{12}(11)$, $\nu_{25}(10)$
1206[a]	1206[a]	1209 (26)	**II**	$\delta_{13}(28)$, $\delta_{12}(17)$, $\nu_5(10)$
		1209 (21)	**IV**	$\delta_{22}(19)$, $\delta_{13}(12)$, $\nu_{25}(11)$, $\nu_{23}(10)$
		1209 (14)	**VI**	$\delta_{27}(28)$, $\nu_{23}(15)$, $\delta_{13}(13)$
		1208 (19)	**I**	$\delta_{13}(27)$, $\delta_{12}(15)$, $\nu_5(11)$
		1208 (31)	**III**	$\delta_{22}(25)$, $\delta_{13}(12)$, $\nu_{25}(11)$
		1208 (17)	**V**	$\delta_{27}(28)$, $\nu_{23}(15)$, $\delta_{13}(12)$
1191[a]	1194[a]	1199 (6)	**I**	$\delta_{27}(36)$, $\delta_{22}(32)$

		1198 (2)	**II**	$\delta_{22}(36)$, $\delta_{27}(34)$
		1196 (5)	**V**	$\delta_{22}(67)$, $\nu_{25}(10)$
		1196 (4)	**VI**	$\delta_{22}(68)$, $\nu_{25}(10)$
		1195 (5)	**IV**	$\delta_{27}(67)$
		1194 (7)	**III**	$\delta_{27}(65)$
	1192[a]	1191 (7)	**I**	$\delta_{22}(34)$, $\delta_{27}(20)$
		1190 (7)	**II**	$\delta_{22}(30)$, $\delta_{27}(22)$
	1189[a]	1188 (1)	**IV**	$\nu_{2}(18)$, $\delta_{12}(10)$
1180 (39.1)	1180[a]	1183 (6)	**I**	$\delta_{13}(17)$, $\nu_{2}(13)$, $\delta_{27}(10)$, $\delta_{12}(10)$, $\delta_{11}(10)$
		1183 (5)	**II**	$\nu_{2}(14)$, $\delta_{13}(14)$, $\delta_{27}(11)$, $\delta_{12}(11)$
		1182 (21)	**III**	$\delta_{22}(30)$
		1182 (15)	**IV**	$\delta_{22}(27)$
	1176[a,b]	1181 (19)	**V**	$\delta_{27}(30)$
		1181 (15)	**VI**	$\delta_{27}(29)$
1156 (21.3)	1159[a,b]	1166 (8)	**I**	$\delta_{10}(33)$, $\delta_{11}(22)$, $\gamma_{7}(13)$, $\gamma_{6}(12)$
		1166 (5)	**II**	$\delta_{10}(34)$, $\delta_{11}(24)$, $\gamma_{7}(14)$, $\gamma_{6}(13)$
		1165 (1)	**V**	$\delta_{10}(34)$, $\delta_{11}(22)$, $\gamma_{7}(13)$, $\gamma_{6}(13)$
		1165 (1)	**VI**	$\delta_{10}(35)$, $\delta_{11}(24)$, $\gamma_{7}(14)$, $\gamma_{6}(14)$
		1161 (14)	**III**	$\delta_{10}(30)$, $\delta_{11}(17)$, $\gamma_{7}(11)$, $\gamma_{6}(10)$
		1161 (8)	**IV**	$\delta_{10}(30)$, $\delta_{11}(19)$, $\gamma_{7}(11)$, $\gamma_{6}(11)$
	1153[a,b]	1159 (1)	**IV**	$\delta_{28}(83)$
		1158 (1)	**IV**	$\delta_{23}(85)$
		1157 (1)	**III**	$\delta_{23}(89)$
1146 (100)	1145 (100)	1161 (49)[d]	**II**	$\delta_{13}(17)$, $\delta_{12}(15)$, $\nu_{16}(14)$
		1160 (78)[d]	**I**	$\nu_{16}(17)$, $\delta_{13}(12)$, $\delta_{12}(10)$
		1159 (41)[d]	**IV**	$\nu_{23}(13)$, $\nu_{26}(12)$, $\nu_{16}(10)$
		1158 (62)[d]	**III**	$\nu_{23}(13)$, $\nu_{26}(12)$, $\nu_{16}(11)$, $\nu_{15}(10)$
		1157 (19)[d]	**VI**	$\delta_{13}(23)$, $\delta_{12}(22)$, $\nu_{16}(16)$
		1157 (36)[d]	**V**	$\nu_{16}(17)$, $\nu_{25}(12)$, $\nu_{15}(10)$
1105 (22.7)	1103 (16.6)	1126 (9)[d]	**VI**	$\nu_{15}(29)$, $\nu_{16}(26)$, $\delta_{12}(12)$
		1128 (37)[d]	**II**	$\nu_{15}(30)$, $\nu_{16}(27)$, $\delta_{12}(10)$
		1128 (11)[d]	**IV**	$\nu_{15}(27)$, $\nu_{16}(25)$
		1127 (11)[d]	**III**	$\nu_{15}(26)$, $\nu_{16}(23)$, $\delta_{12}(11)$

		1126 (25)[d]	**I**	$\nu_{15}(27)$, $\nu_{16}(23)$, $\delta_{12}(13)$
		1125 (12)[d]	**V**	$\nu_{15}(28)$, $\nu_{16}(23)$, $\delta_{12}(14)$
1090 (20.0)	1091 (22.8)	1113 (3)	**IV**	$\delta_{13}(40)$, $\delta_{12}(34)$
		1110 (4)	**III**	$\delta_{13}(39)$, $\delta_{12}(32)$
		1110 (5)	**V**	$\delta_{13}(28)$, $\delta_{12}(25)$
		1108 (14)	**I**	$\delta_{12}(21)$, $\delta_{13}(21)$
		1107 (9)	**II**	$\delta_{13}(30)$, $\delta_{12}(27)$
1051 (16.3)	1050 (19.1)	1055 (27)	**I**	$\delta_{17}(35)$, $\nu_{27}(12)$
		1055 (22)	**II**	$\delta_{17}(35)$, $\nu_{27}(11)$
		1054 (12)	**III**	$\delta_{17}(31)$, $\nu_{26}(12)$
		1054 (8)	**IV**	$\delta_{17}(28)$, $\delta_{18}(17)$, $\nu_{26}(10)$
		1052 (2)	**VI**	$\delta_{18}(39)$, $\delta_{17}(25)$
		1051 (1)	**I**	$\delta_{18}(77)$
		1051 (2)	**II**	$\delta_{18}(71)$
		1051 (1)	**III**	$\delta_{18}(71)$
		1051 (2)	**IV**	$\delta_{18}(61)$
		1051 (1)	**V**	$\delta_{18}(31)$, $\delta_{17}(29)$
		1049 (1)	**V**	$\delta_{18}(49)$, $\delta_{17}(21)$
		1048 (1)	**VI**	$\delta_{18}(40)$, $\delta_{17}(26)$
1003 (3.9)	1001 (3.5)	1001 (3)	**I**	$\nu_{26}(45)$, $\nu_{27}(11)$, $\delta_{17}(10)$
		1001 (2)	**II**	$\nu_{26}(46)$, $\nu_{27}(11)$, $\delta_{17}(10)$
		1001 (2)	**V**	$\nu_{26}(45)$, $\nu_{27}(20)$
		1001 (1)	**VI**	$\nu_{26}(44)$, $\nu_{27}(21)$
989[a,b]		998 (1)	**III**	$\nu_{26}(47)$
		984 (1)	**V**	$\nu_{27}(39)$, $\nu_{26}(13)$
		984 (1)	**VI**	$\nu_{27}(39)$, $\nu_{26}(14)$
977[a]		975 (1)	**III**	$\nu_{27}(53)$
		975 (1)	**IV**	$\nu_{27}(54)$, $\delta_{17}(10)$
967 (3.9)	965 (5.7)	963 (5)	**I**	$\nu_{27}(45)$, $\nu_{26}(13)$
		963 (5)	**II**	$\nu_{27}(46)$, $\nu_{26}(12)$
932 (0.8) *?*				
912 (2.7)	912 (4.0)	917 (1)	**I**	$\nu_{10}(13)$
		910 (2)	**IV**	$\gamma_{9}(24)$, $\gamma_{8}(22)$

		908 (3)	**III**	$\gamma_9(23)$, $\gamma_7(22)$
887 (1.4)	886[a]	890 (1)	**II**	$\gamma_8(32)$, $\gamma_9(32)$
		888 (2)	**I**	$\gamma_8(29)$, $\gamma_9(28)$
		881 (1)	**IV**	$\gamma_8(21)$, $\gamma_9(19)$, $\gamma_6(10)$
870[a,b]		878 (1)	**III**	$\gamma_8(24)$, $\gamma_9(22)$
857 (1.7)		856 (2)	**V**	$\nu_{25}(18)$
		856 (1)	**VI**	$\nu_{25}(19)$
813[a]	817[a]	810 (2)	**VI**	$\delta_3(16)$
		809 (5)	**II**	$\gamma_{11}(17)$, $\delta_3(12)$
		808 (2)	**V**	$\gamma_{11}(17)$, $\delta_3(13)$
807[a,b]	807[a]	807 (4)	**I**	$\gamma_{11}(23)$, $\tau_2(11)$
		805 (3)	**III**	$\gamma_{11}(33)$, $\tau_2(12)$, $\gamma_4(11)$
		805 (2)	**IV**	$\gamma_{11}(32)$
788 (1.4)		795 (1)	**II**	$\gamma_{10}(24)$, $\tau_2(20)$, $\gamma_{11}(16)$, $\gamma_3(14)$, $\gamma_4(10)$
		794 (1)	**V**	$\gamma_{10}(36)$, $\tau_2(15)$, $\gamma_3(14)$
		793 (1)	**I**	$\gamma_{10}(34)$, $\tau_2(13)$, $\gamma_3(13)$
		792 (1)	**III**	$\gamma_{10}(21)$, $\gamma_3(12)$, $\tau_2(12)$
781[a]	776[a]	783 (4)	**I**	$\gamma_{11}(20)$, $\delta_{30}(17)$, $\gamma_{10}(13)$
		783 (1)	**V**	$\gamma_{11}(24)$, $\delta_{30}(16)$, $\delta_{33}(10)$
		782 (4)	**II**	$\gamma_{10}(18)$, $\delta_{30}(17)$, $\gamma_{11}(11)$, $\delta_{30}(10)$
		782 (1)	**VI**	$\gamma_{11}(18)$, $\delta_{30}(18)$, $\delta_{33}(11)$, $\gamma_{10}(10)$
771 (5.8)		776 (2)	**III**	$\delta_{30}(21)$, $\delta_{33}(12)$, $\gamma_{10}(10)$
		775 (1)	**IV**	$\delta_{30}(21)$, $\gamma_{10}(14)$, $\delta_{33}(12)$
		769 (7)	**II**	$\delta_{32}(17)$, $\delta_{34}(10)$
		768 (2)	**IV**	$\delta_{32}(17)$
		767 (1)	**VI**	$\delta_{32}(20)$, $\delta_{34}(11)$
		766 (3)	**III**	$\delta_{32}(15)$
		766 (8)	**I**	$\delta_{32}(15)$
		765 (2)	**V**	$\delta_{32}(18)$, $\delta_{34}(10)$
752 (4.9)	752[a]	746 (1)	**I**	$\nu_{11}(11)$, $\gamma_{11}(11)$
		744 (2)	**II**	$\nu_{11}(12)$, $\gamma_{10}(11)$, $\gamma_{11}(10)$, $\nu_{14}(10)$
		743 (1)	**III**	$\nu_{11}(12)$, $\gamma_{11}(11)$
		741 (1)	**IV**	$\gamma_{10}(14)$, $\nu_{11}(13)$, $\nu_{14}(10)$, $\gamma_{11}(10)$

668 (9.4)	669[a]	669 (1)	**III**	$\nu_{14}(31)$, $\delta_4(16)$, $\tau_2(13)$
		666 (3)	**I**	$\tau_2(24)$, $\nu_{14}(24)$, $\delta_4(14)$
		666 (1)	**IV**	$\nu_{14}(40)$, $\delta_4(15)$
		665 (1)	**VI**	$\tau_2(22)$, $\tau_1(12)$, $\gamma_4(10)$
		662 (3)	**II**	$\nu_{14}(27)$, $\tau_2(16)$
		661 (2)	**V**	$\nu_{14}(29)$, $\tau_1(21)$
		659 (3)	**I**	$\tau_1(24)$, $\gamma_5(11)$, $\tau_2(11)$, $\gamma_4(10)$
		659 (1)	**III**	$\tau_1(22)$, $\tau_2(12)$, $\gamma_5(11)$, $\nu_{11}(10)$, $\gamma_4(10)$
		643 (1)	**IV**	$\tau_2(33)$
		641 (1)	**I**	$\tau_2(28)$, $\nu_{11}(28)$
		640 (3)	**II**	$\tau_2(32)$
		639 (1)	**V**	$\tau_2(30)$, $\nu_{11}(25)$
		636 (1)	**VI**	$\tau_2(32)$
		627 (1)	**II**	$\tau_1(48)$, $\gamma_5(11)$
		624 (1)	**VI**	$\tau_1(48)$, $\gamma_5(11)$
		617 (1)	**I**	$\tau_1(42)$, $\gamma_5(10)$
		614 (1)	**V**	$\tau_1(43)$, $\gamma_5(12)$
597[a]	598[a]	593 (1)	**III**	$\delta_2(40)$, $\nu_{10}(18)$
		593 (1)	**V**	$\delta_2(35)$, $\nu_{10}(17)$
		592 (2)	**I**	$\delta_2(38)$, $\nu_{10}(18)$
		592 (1)	**IV**	$\delta_2(38)$, $\nu_{10}(16)$
		591 (2)	**II**	$\delta_2(37)$, $\nu_{10}(17)$
572 (29.9)	575[a]	558 (2)	**VI**	$\delta_4(28)$, $\gamma_1(20)$
		556 (4)	**IV**	$\delta_4(29)$, $\gamma_1(21)$
		555 (10)	**II**	$\delta_4(30)$, $\gamma_1(22)$
		553 (6)	**III**	$\delta_4(29)$, $\gamma_1(23)$
		553 (3)	**V**	$\delta_4(28)$, $\gamma_1(24)$
		551 (12)	**I**	$\delta_4(30)$, $\gamma_1(25)$
466 (8.2)		457 (2)	**V**	$\delta_{31}(21)$
		460 (2)	**VI**	$\delta_{31}(20)$
452[a]		452 (4)	**III**	$\gamma_2(23)$, $\delta_{29}(17)$
		451 (4)	**II**	$\delta_5(17)$, $\delta_6(15)$, $\delta_8(13)$, $\delta_{31}(11)$
		450 (5)	**I**	$\delta_6(14)$, $\delta_5(14)$, $\delta_3(13)$, $\delta_{29}(10)$

	450 (3)	**IV**	$\gamma_2(23)$, $\delta_{29}(16)$
	447 (2)	**IV**	$\delta_{31}(18)$, $\delta_5(16)$, $\delta_6(14)$, $\delta_3(10)$
	444 (3)	**III**	$\delta_{31}(17)$, $\delta_5(15)$, $\delta_6(14)$, $\delta_3(10)$
	444 (1)	**V**	$\delta_{29}(19)$, $\gamma_2(14)$, $\delta_5(10)$
	442 (1)	**VI**	$\delta_{29}(18)$, $\gamma_2(15)$, $\delta_5(10)$
	436 (3)	**II**	$\gamma_2(26)$
	435 (3)	**I**	$\gamma_2(25)$
415[a]	408 (3)	**II**	$\delta_{31}(30)$, $\delta_{29}(18)$, $\nu_2(10)$
	407 (4)	**I**	$\delta_{31}(30)$, $\delta_{29}(17)$
	403 (2)	**III**	$\delta_{31}(19)$, $\delta_5(11)$
	401 (2)	**IV**	$\delta_{31}(22)$, $\delta_5(12)$

[a] bands overlaid or of low intensity, calculation of integration not possible, [b] shoulder, [c] the theoretical bands of relative intensity ≥ 0.5 km/mol are included, frequencies scaled by factor of 0.990, unless denoted by superscript, [d] frequencies scaled by factor of 1.035, [e] PED contribution ≥ 10 % are given.

Table 4S. IR frequencies (in cm^{-1}) observed in the spectra of amorphous (ν_{amorph}) and crystalline state (ν_{cryst}) of PTD with the assignment of the crystalline state based on calculated frequencies (ν_{calc}) of conformer **VI**.

ν_{amorph} (cm^{-1})	ν_{cryst} (cm^{-1})	ν_{calc} (cm^{-1})[b]	Assignment[d]
2998 m	3032 m	3129 (1)	$\nu_{19}(93)$
		3128 (13)	$\nu_{31}(81)$, $\nu_{32}(11)$
		3122 (14)	$\nu_{28}(79)$, $\nu_{30}(11)$
		3114 (5)	$\nu_{12}(80)$, $\nu_{13}(19)$
	3004 m	3093 (18)	$\nu_{32}(51)$, $\nu_{33}(48)$
		3092 (17)	$\nu_{30}(51)$, $\nu_{29}(48)$
2956 m	2966 m	3041 (4)	$\nu_{13}(81)$, $\nu_{12}(18)$
		3036 (11)	$\nu_{18}(69)$, $\nu_{17}(29)$
		3031 (12)	$\nu_{20}(54)$, $\nu_{21}(46)$
		3021 (39)	$\nu_{33}(44)$, $\nu_{32}(37)$, $\nu_{31}(18)$
		3020 (38)	$\nu_{29}(42)$, $\nu_{30}(37)$, $\nu_{28}(20)$
	2945 m	2989 (27)	$\nu_{21}(51)$, $\nu_{20}(43)$
~2855[a] vw			
~2722 vw			
1705 vs	1725 s	1763 (335)	$\nu_{24}(79)$
	1716 s	1723 (273)	$\nu_{22}(76)$
	1705 s		
1584 w	1597 w	1591 (64)	$\nu_{1}(50)$, $\nu_{5}(11)$, $\nu_{8}(10)$
1548 m	1547 m	1548 (86)	$\nu_{8}(42)$, $\nu_{10}(11)$, $\nu_{1}(10)$
1450 s	1460 s	1485 (6)	$\delta_{21}(62)$, $\delta_{20}(14)$, $\delta_{22}(10)$
		1481 (4)	$\delta_{15}(43)$, $\gamma_{6}(18)$, $\gamma_{7}(18)$
		1481 (8)	$\delta_{26}(59)$, $\delta_{25}(18)$, $\delta_{27}(11)$
		1475 (13)	$\delta_{15}(46)$, $\gamma_{6}(12)$, $\delta_{16}(12)$, $\gamma_{7}(12)$
		1469 (6)	$\delta_{16}(51)$
		1468 (10)	$\delta_{25}(70)$, $\delta_{26}(19)$
		1467 (7)	$\delta_{20}(67)$, $\delta_{21}(16)$
	1455	1460 (50)	$\delta_{24}(63)$
		1455 (34)	$\delta_{19}(68)$, $\delta_{24}(10)$
	1448 s	1443 (9)	$\gamma_{8}(41)$, $\gamma_{9}(38)$
1418 m	1420 m	1426 (148)	$\nu_{2}(22)$
	1402 m	1408 (19)	$\delta_{14}(67)$
1397 m	1396 m	1398 (35)	$\nu_{4}(26)$, $\delta_{14}(17)$, $\nu_{7}(10)$
~1390[a] m	1389 m	1382 (23)	$\nu_{6}(32)$, $\delta_{1}(18)$
	~1379[a] w		
1342 s	1329 s	1351 (205)[c]	$\nu_{16}(43)$, $\nu_{15}(39)$
1309 s	1309 s	1310 (240)	$\nu_{23}(17)$, $\nu_{3}(17)$, $\nu_{9}(11)$
~1252[a] s	1256 w	1246 (109)	$\delta_{11}(30)$, $\delta_{10}(22)$
	1227 m	1216 (91)	$\delta_{13}(15)$, $\delta_{12}(11)$, $\nu_{25}(10)$
1209 s	1213 s	1209 (204)	$\delta_{27}(28)$, $\nu_{23}(15)$, $\delta_{13}(13)$
	1201 m	1196 (52)	$\delta_{22}(68)$, $\nu_{25}(10)$
1183 m	1177 m	1184 (1)	$\nu_{7}(13)$, $\delta_{13}(13)$, $\nu_{2}(11)$, $\delta_{12}(11)$, $\delta_{2}(10)$
		1181 (221)	$\delta_{27}(29)$
	1162 w	1165 (9)	$\delta_{10}(35)$, $\delta_{11}(24)$, $\gamma_{7}(14)$, $\gamma_{6}(14)$
		1157 (276)[c]	$\delta_{13}(23)$, $\delta_{12}(22)$, $\nu_{16}(16)$
		1159 (1)	$\delta_{23}(91)$
		1158 (1)	$\delta_{28}(91)$
1145 s	1140 s	1126 (131)[c]	$\nu_{15}(29)$, $\nu_{16}(26)$, $\delta_{12}(12)$
~1106[a] m	~1102[a] m	1107 (163)	$\delta_{13}(12)$, $\delta_{12}(11)$, $\nu_{25}(11)$
1095 m	1095 m		
1052 m	1053 m	1052 (22)	$\delta_{18}(39)$, $\delta_{17}(25)$
	1047 w	1048 (11)	$\delta_{18}(40)$, $\delta_{17}(26)$

	1041 w		
996 w	991 w	1001 (15)	$\nu_{26}(44)$, $\nu_{27}(21)$
963 w	969 vw	984 (8)	$\nu_{27}(39)$, $\nu_{26}(14)$
	933 vw	928 (1)	$\gamma_6(33)$, $\gamma_7(33)$
916 w	907 w	885 (1)	$\gamma_8(27)$, $\gamma_9(25)$
~891[a] w			
861 w	863 w	856 (19)	$\nu_{25}(19)$
	~827[a] w		
815 w	817 m	810 (24)	$\delta_3(16)$
~787[a] m	784 w	794 (7)	$\gamma_{10}(28)$, $\tau_2(21)$, $\gamma_3(15)$, $\gamma_{11}(14)$, $\gamma_3(10)$
779 m	778 m	782 (13)	$\gamma_{11}(18)$, $\delta_{30}(18)$, $\delta_{33}(11)$, $\gamma_{10}(10)$
~772[a] m			
751 w	752 w	767 (15)	$\delta_{32}(20)$, $\delta_{34}(11)$
		741 (6)	$\gamma_{10}(12)$, $\nu_{11}(12)$, $\gamma_{11}(12)$
700 vw			
670 w	668 vw	665 (12)	$\tau_2(22)$, $\tau_1(12)$, $\gamma_4(10)$
	658 vw	659 (2)	$\nu_{14}(32)$, $\nu_{11}(27)$, $\delta_4(21)$
	650 vw		
	640 vw	636 (14)	$\tau_2(32)$
639 wv	620 vw	624 (8)	$\tau_1(48)$, $\gamma_5(11)$
598 w	600 w	593 (6)	$\delta_2(33)$, $\nu_{10}(16)$
576 m	581 m	558 (30)	$\delta_4(28)$, $\gamma_1(20)$
	470 m	460 (27)	$\delta_{31}(20)$
		442 (12)	$\delta_{29}(18)$, $\gamma_2(15)$, $\delta_5(10)$

[a]shoulder, [b] calculations at B3LYP/6-311++G(d,p), integral intensities given in parentheses (in km/mol), the theoretical bands of relative intensity ≥ 0.5 km/mol are included frequencies scaled by factor of 0.990, unless denoted by superscript, [c] frequencies scaled by factor of 1.035 , [d] PED contribution ≥ 10 % are given.