Electronic Supporting Information for

Pyrrolo[*3,4-c*]pyridine-1,2-dione: A New Electron Acceptor for Electrochromic Conjugated Polymers

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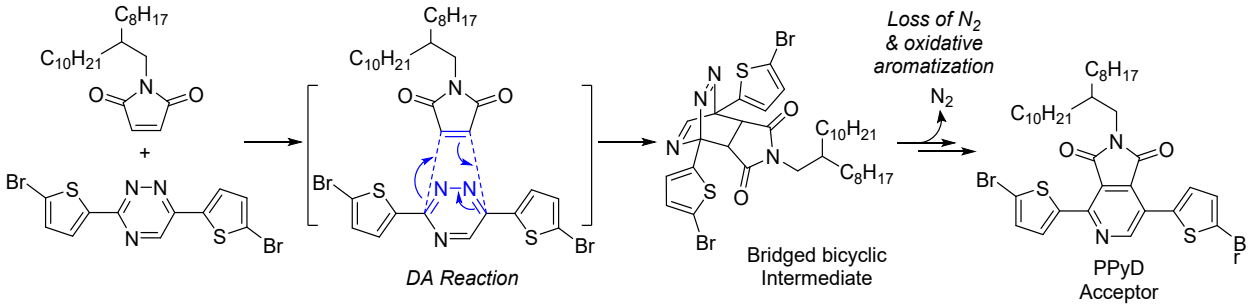
Correspondence: jw-xu@imre.a-star.edu.sg (J. Xu), david.j.procter@manchester.ac.uk (D.J. Procter)

Content:

1. Mechanism and chemical characterization



Scheme S1. Proposed mechanism for synthesis of PPyD acceptor

2. Optical and electrochemical properties

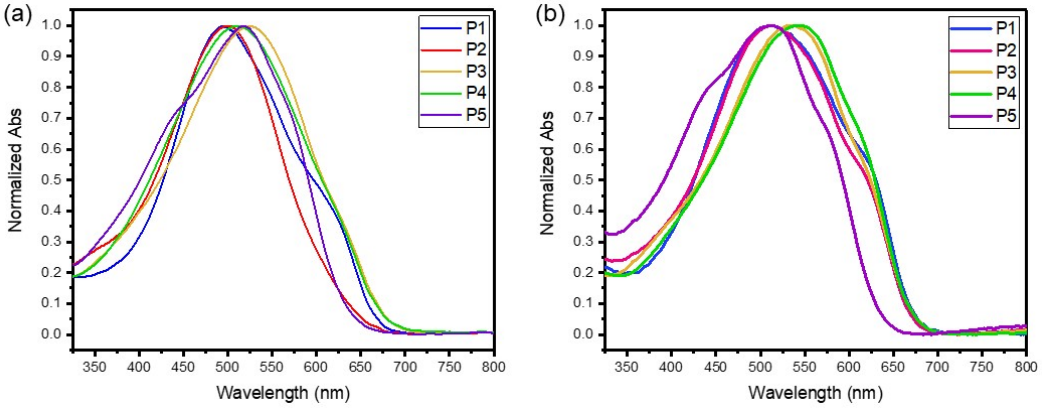


Figure S1. Normalized UV-Vis absorption spectra of polymers **P1** – **P5** in dilute solution (a) and thin film state (b).

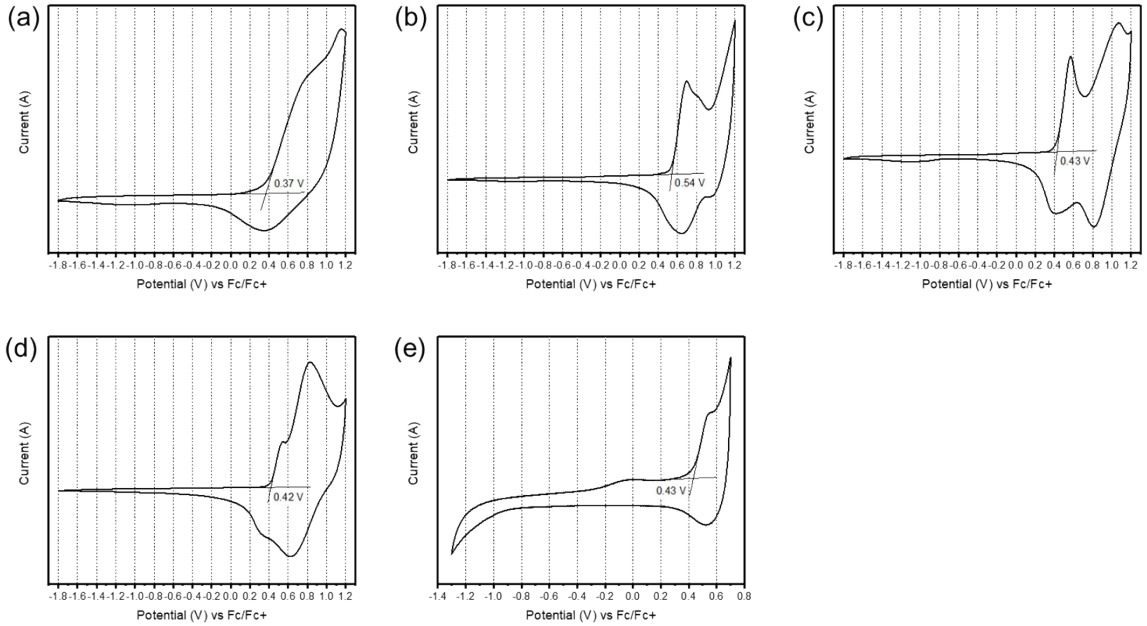


Figure S2. Normalized cyclic voltammograms of polymers (a) **P1** (b) **P2**, (c) **P3**, (d) **P4** and (e) **P5** in performed in 0.1M $LiClO_4$/ACN electrolyte, with glassy carbon working electrode, silver wire reference electrode and platinum wire counter electrode, calibrated against ferrocene reference.

3. DFT Calculations

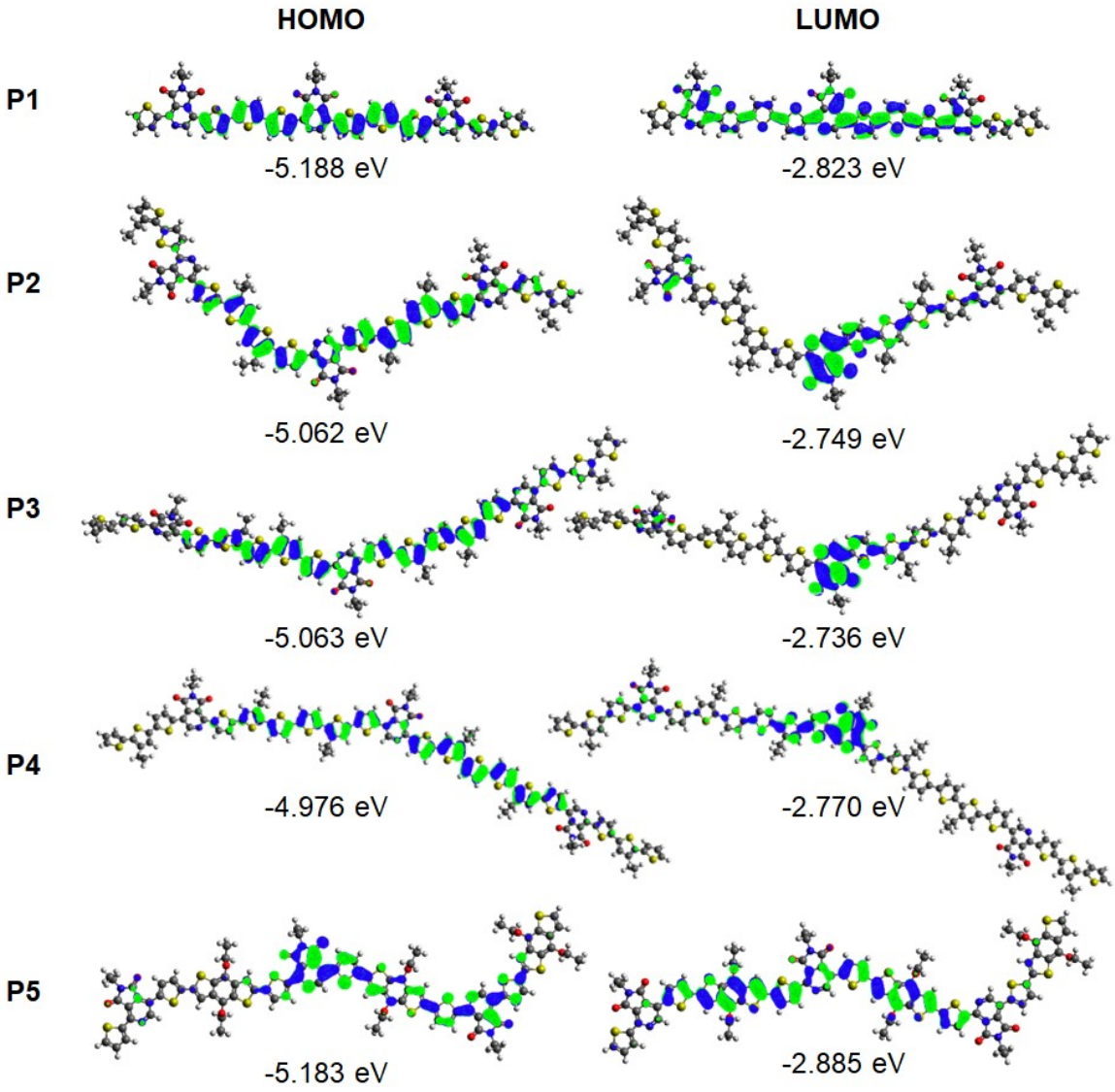
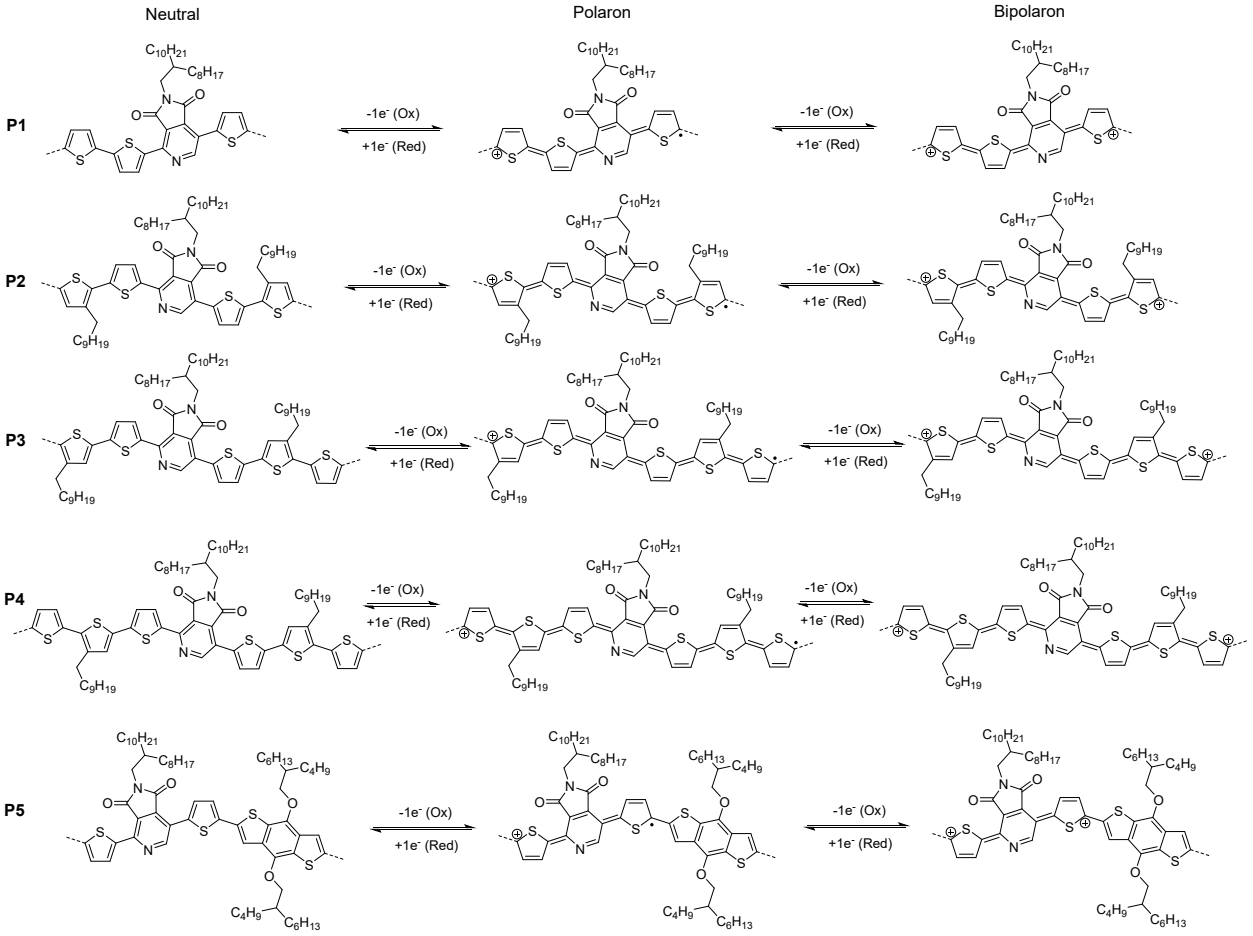


Figure S3. Optimized geometries (top), and HOMO and LUMO coefficients distribution of 3 repeating units of **P1** – **P5**, with the respective HOMO and LUMO energy levels stated. For simplicity, all long and branched alkyl chains were replaced with short ethyl groups. Calculations were done at B3LYP/def2-TZVP level with SMD solvation model used (solvent = diphenylether) and temperature at 463.15K.

Reference:

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

4. Spectroelectrochemistry Mechanism



Scheme S2. Proposed mechanism of electrochromism in **P1** to **P5**, in which polarons and bipolarons were formed upon undergoing electrochemical oxidation.

5. Colourimetric Analysis

Table S1. CIE 1976 *L*a*b** colour space colour coordinates of polymers **P1** – **P5** at different applied voltages.

Polymer	Applied Voltage	*L**	*a**	*b**
P1	0.0 V	71.24	14.93	-5.61
	1.6 V	73.09	9.93	-9.15
	2.0 V	76.24	2.42	-9.69
	2.4 V	78.04	1.19	-6.89
P2	0.0 V	71.26	17.26	-5.41
	1.7 V	80.23	1.04	-5.04
	2.0 V	84.38	-0.4	-1.33
	2.4 V	81.23	0.47	-2.64
P3	0.0 V	68.24	18.77	-11.05
	1.6 V	78.96	-2.05	-6.4
	2.0 V	80.5	-4.73	-6.15
	2.4 V	82.76	-4.23	-2.98
P4	0.0 V	64.58	19.09	-14.04
	1.5 V	77.7	-0.97	-6.65
	2.0 V	82.26	-3.74	-5.15
	2.4 V	83.37	-3.34	-3.39
P5	0.0 V	77.44	17.79	5.22
	1.8 V	79.6	8.66	8.09
	2.4 V	83.62	3.74	14.86

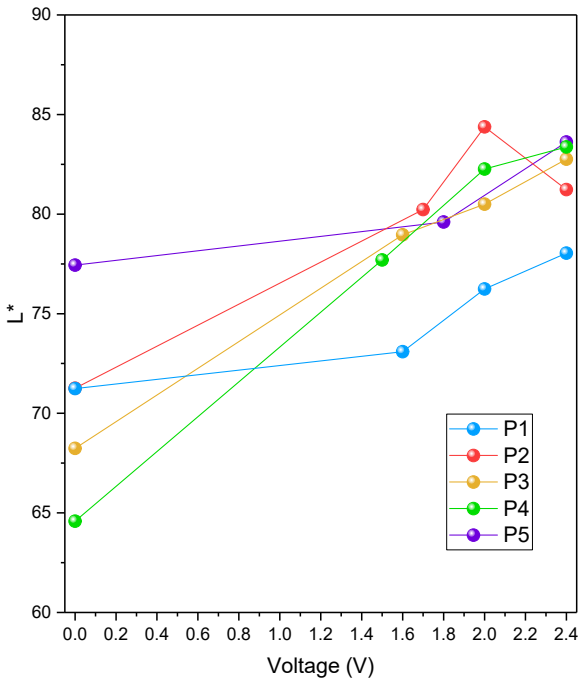


Figure S4. (Plot of *L** values of polymers **P1** – **P5** against applied voltages.

6. Chronoabsorptometry (EC switching) studies

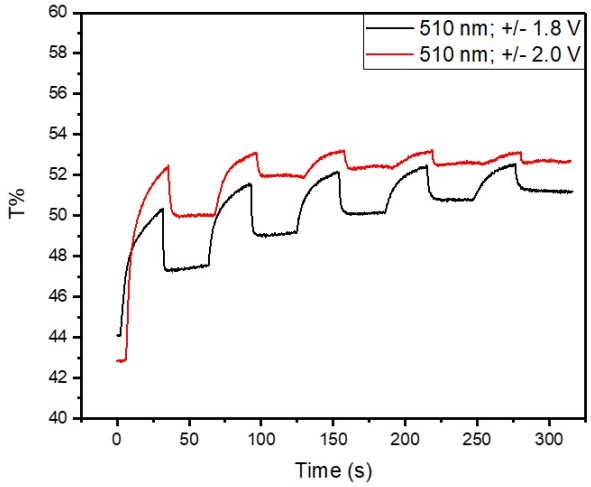


Figure S5. Chronoabsorptometry studies into the transmittance change of polymer **P5** at 510 nm performed at +/- 1.8 and +/- 2.0 V at 40 s time interval.

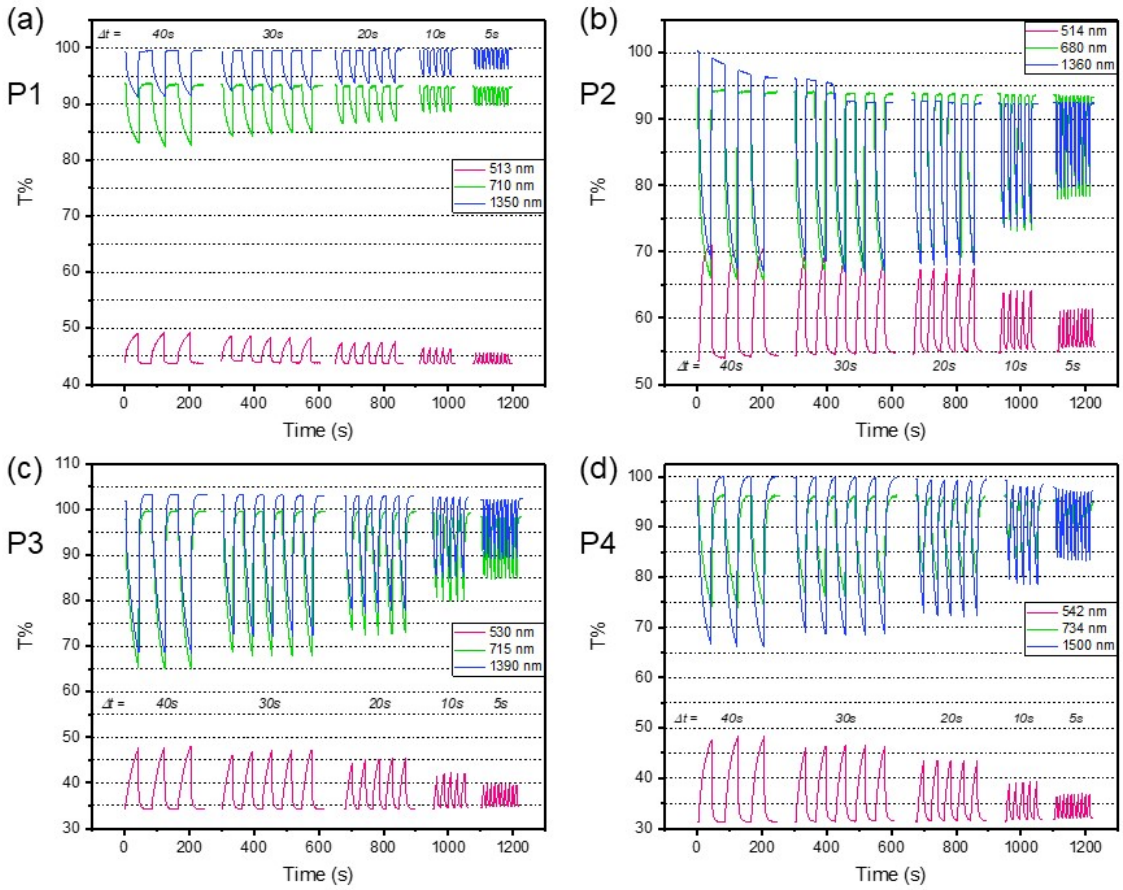


Figure S6. Chronoabsorptometry studies into the transmittance changes to the visible, far-red and NIR wavelengths of study of polymers **P1** (a), **P2** (b), **P3** (c) and **P4** (d) performed at +/- 1.6, +/- 1.7, +/-1.6 and +/-1.5 V, respectively, at different time intervals (Δt) of 40, 30, 20, 10 and 5 s.

Table S2. Optical contrasts of polymers **P1**, **P2**, **P3** and **P4**, based on chronoabsorptometry studies performed at +/- 1.6, +/- 1.7, +/-1.6 and +/-1.5 V, respectively, at different time intervals (Δt) of 40, 30, 20, 10 and 5 s.

Polymer	Wavelength (nm)	Optical Contrast				
		Δt = 40 s	Δt = 30 s	Δt = 20 s	Δt = 10 s	Δt = 5 s
P1	513 nm	5.5 %	4.7 %	3.7 %	2.7 %	1.7 %
	710 nm	11.2 %	8.7 %	6.4 %	4.7 %	3.3 %
	1350 nm	8.1 %	7.1 %	6.0 %	4.7 %	3.6 %
P2	514 nm	16.6 %	12.5 %	12.7 %	8.9 %	5.7 %
	680 nm	28.6 %	27.0 %	24.7 %	20.4 %	14.0 %
	1360 nm	29.5 %	27.3 %	24.7 %	18.7 %	13.2 %
P3	530 nm	13.7 %	12.9 %	11.1 %	7.8 %	5.0 %
	715 nm	34.7 %	31.8 %	26.9 %	19.1 %	13.2 %
	1390 nm	34.7 %	31.1 %	25.5 %	17.6 %	12.9 %
P4	542 nm	16.9 %	15.1 %	12.0 %	7.5 %	4.8 %
	734 nm	22.5 %	19.9 %	16.6 %	11.6 %	8.2 %
	1500 nm	33.8 %	31.4 %	27.1 %	19.7 %	13.8 %

Table S3. Optical contrasts of polymers **P1**, **P2**, **P3** and **P4**, based on chronoabsorptometry studies performed at +/- 2.0, +/- 1.9, +/-1.9 and +/- 2.0 V, respectively, at different time intervals (Δt) of 40, 30, 20, 10 and 5 s.

Polymer	Wavelength (nm)	Optical Contrast				
		Δt = 40 s	Δt = 30 s	Δt = 20 s	Δt = 10 s	Δt = 5 s
P1	513 nm	11.4 %	10.4 %	9.2 %	6.6 %	4.2 %
	1350 nm	21.4 %	21.6 %	18.2 %	14.3 %	9.7 %
P2	514 nm	20.5 %	18.5 %	14.4 %	10.0 %	6.8 %
	1360 nm	30.9 %	28.1 %	24.7 %	20.4 %	14.0 %
P3	530 nm	28.5 %	26.8 %	23.2 %	18.1 %	12.0 %
	1390 nm	46.8 %	42.1 %	37.0 %	30.4 %	19.6 %
P4	542 nm	35.6 %	33.6 %	32.6 %	30.6 %	27.1 %
	1500 nm	69.4 %	62.3 %	59.4 %	55.7 %	51.5 %

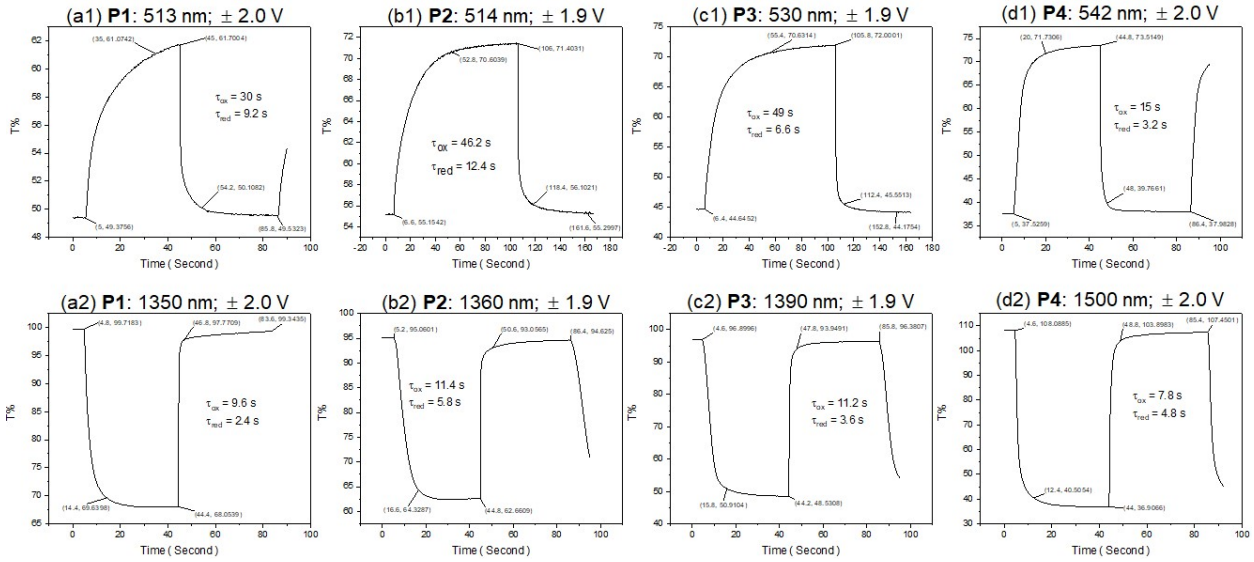


Figure S7. Measurement and determination of switching speeds for **P1** (a1, a2), **P2** (b1, b2), **P3** (c1, c2) and **P4** (d1, d2). τ_{ox} and τ_{red} refer to the switching speed for the oxidation and reduction process, respectively, and refer to bleaching and colouration time, τ_b and τ_c, respectively.

7. EC switching stability studies

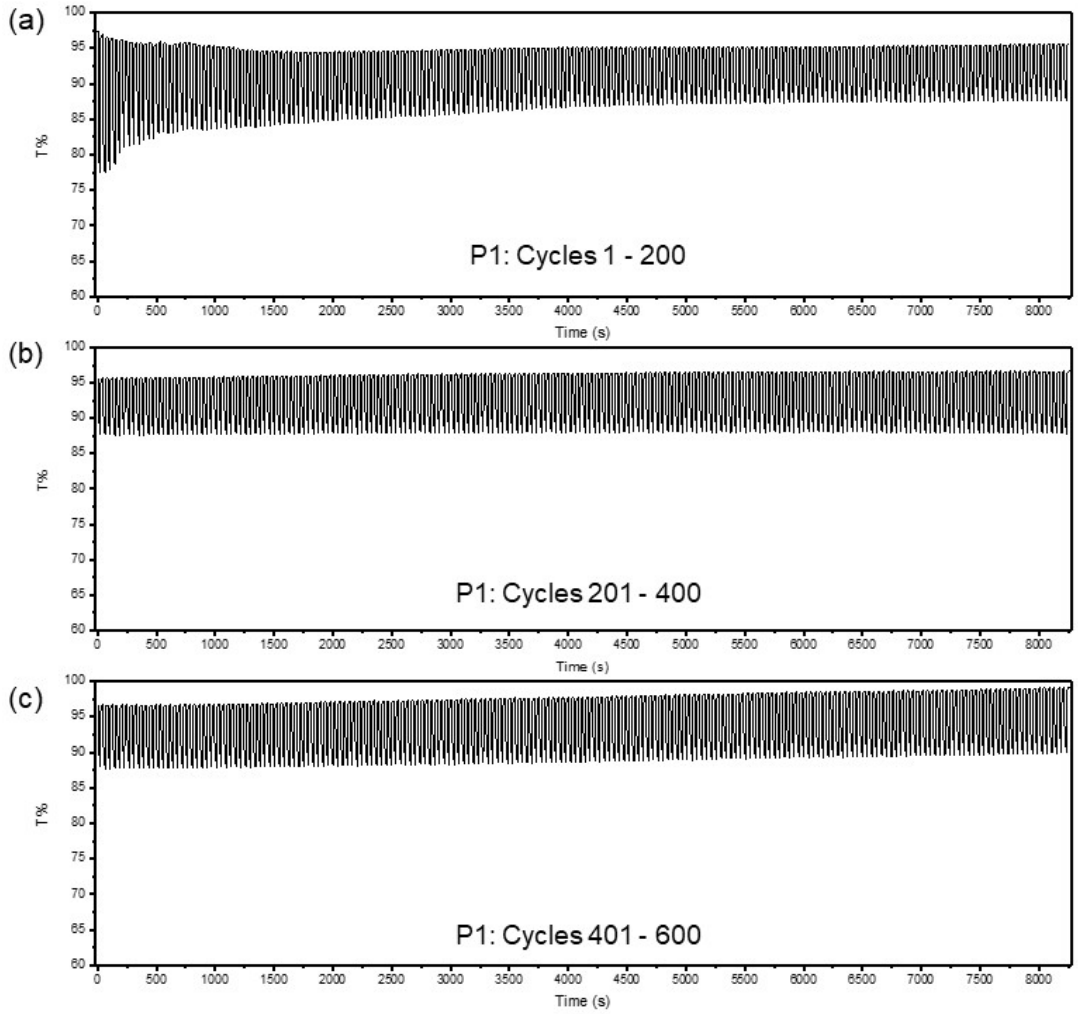


Figure S8. EC switching of polymer **P1** at 1350 nm with applied voltage of +/- 2.0 V at 20 s time interval, from cycles 1 – 200 (a), cycles 201 – 400 (b) and cycles 401 – 600 (c).

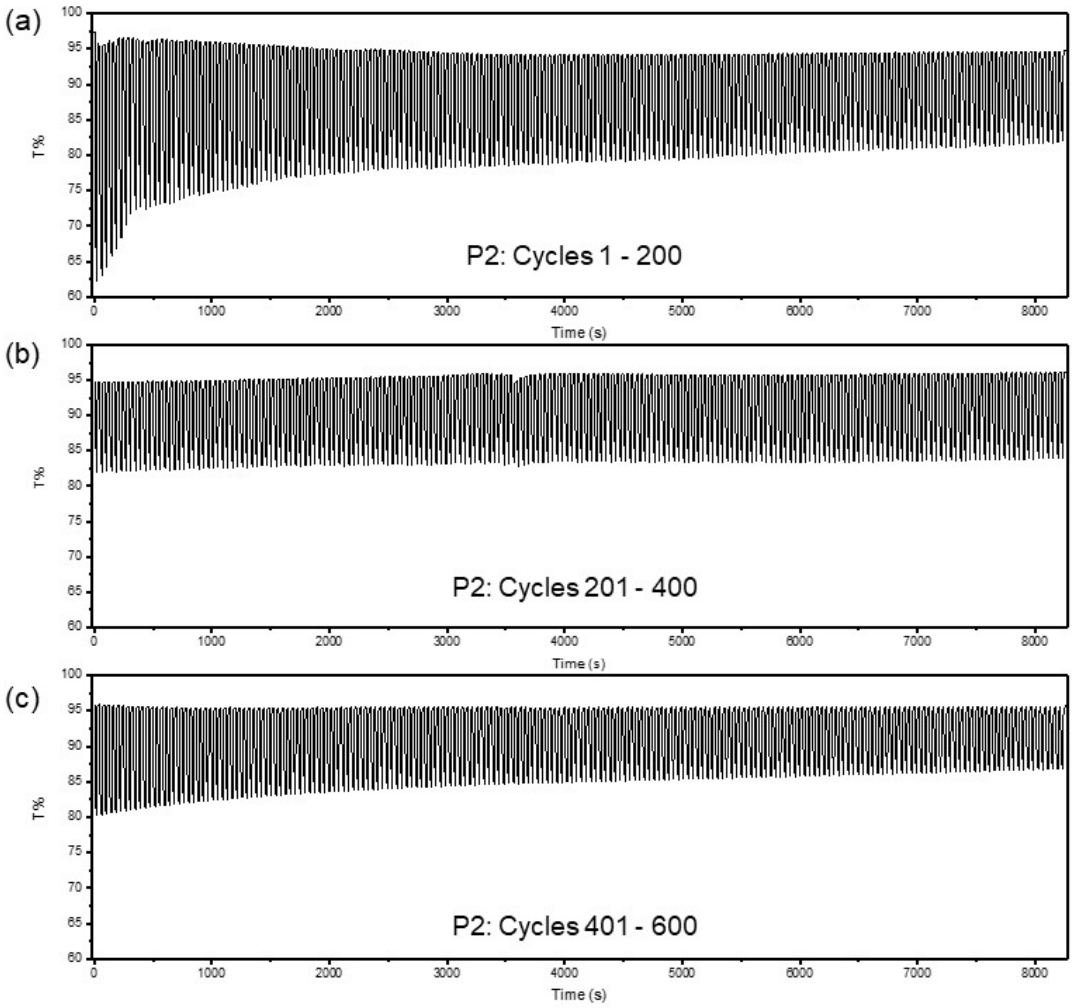


Figure S9. EC switching of polymer **P2** at 1360 nm with applied voltage of +/- 1.9 V at 20 s time interval, from cycles 1 – 200 (a), cycles 201 – 400 (b) and cycles 401 – 600 (c).

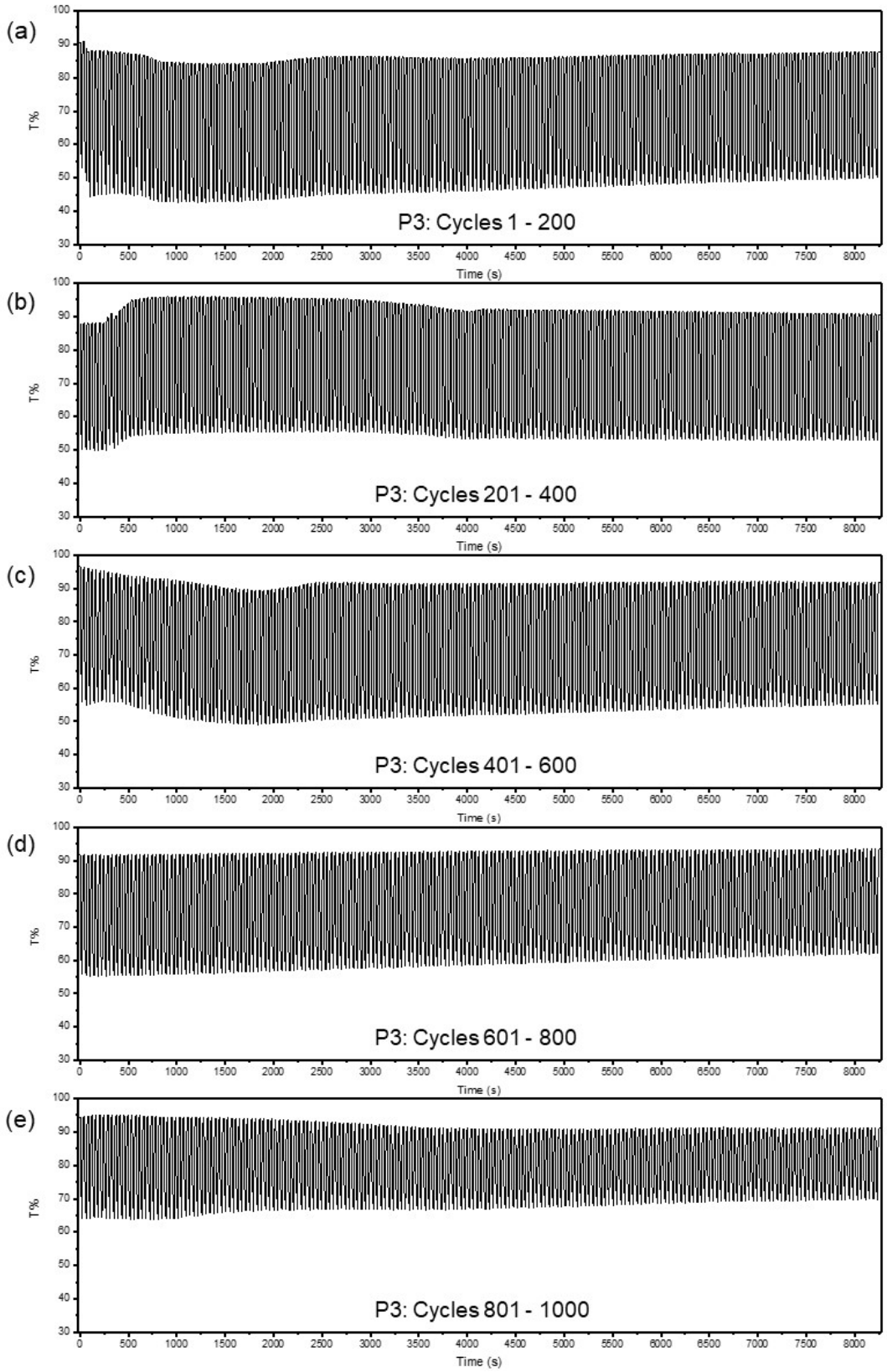


Figure S10. EC switching of polymer **P3** at 1390 nm with applied voltage of +/- 1.9 V at 20 s time interval, from cycles 1 – 200 (a), cycles 201 – 400 (b), cycles 401 – 600 (c), cycles 601 – 800 (d) and cycles 801 – 1000 (e).

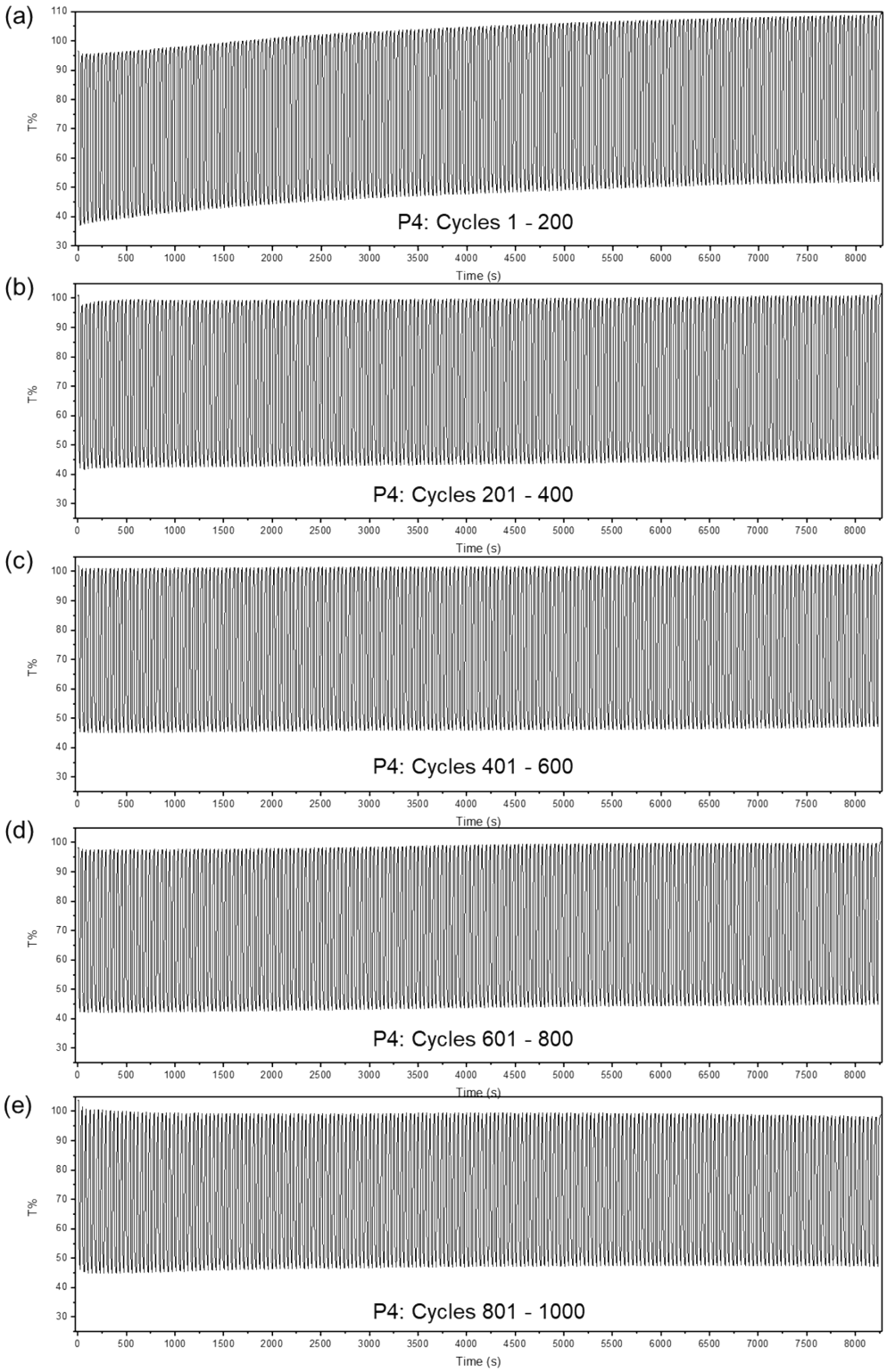
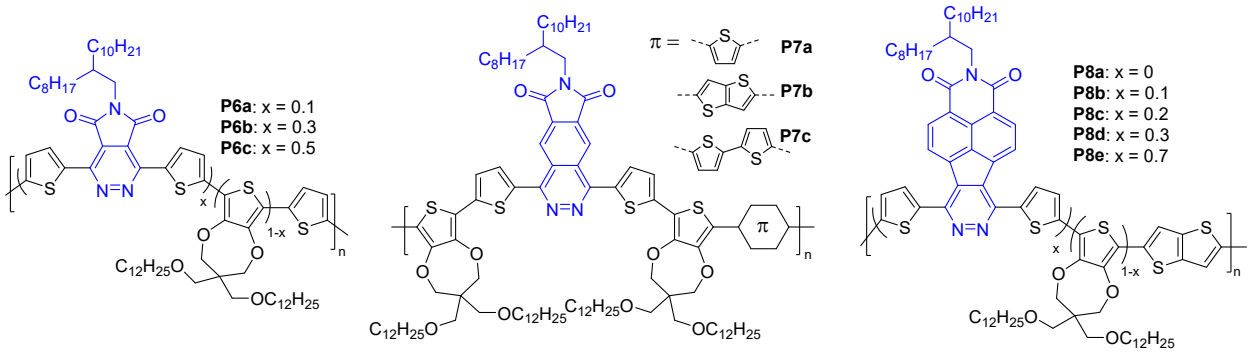


Figure S11. EC switching of polymer **P4** at 1500 nm with applied voltage of +/- 2.0 V at 20 s time interval, from cycles 1 – 200 (a), cycles 201 – 400 (b), cycles 401 – 600 (c), cycles 601 – 800 (d) and cycles 801 – 1000 (e).

8. Comparison of EC performance with analogous EC polymers



Pyrrolo[3,4-d]pyridazine dione -based EC Polymers

Pyrrolophthalazine dione (PPD) -based EC Polymers

Pyrrolo-acenaphtho-pyridazine Dione (PAPD) -based EC Polymers

Scheme S3. Chemical structures of EC donor-acceptor type polymers with structurally analogous acceptor groups.

Table S4. Comparison of EC switching properties of PPyD-based polymers **P1** – **P4** with that of polymers with structurally analogous acceptor groups (**P6a** – **P8e**).

	Colour Change		Visible				NIR			
	Neutral Colour	Oxidised Colour	λ_{abs} (nm)	Max. OC (%)	τ (s)	CE ($cm^2\ C^{-1}$)	λ_{abs} (nm)	Max. OC (%)	τ (s)	CE ($cm^2\ C^{-1}$)
PPyD -based EC Polymers (This Work)										
P1	Wine Red	Purplish Blue	513	12.2	$\tau_b = 30.0$ $\tau_c = 9.2$	79	1350	31.6	$\tau_b = 9.6$ $\tau_c = 2.4$	205
P2	Wine Red	Purplish Blue	514	20.5	$\tau_b = 46.2$ $\tau_c = 12.4$	203	1360	32.0	$\tau_b = 11.4$ $\tau_c = 5.8$	377
P3	Magenta	Cyan	530	28.5	$\tau_b = 49.0$ $\tau_c = 6.6$	294	1390	48.4	$\tau_b = 11.2$ $\tau_c = 3.6$	590
P4	Magenta	Cyan	542	35.6	$\tau_b = 15.0$ $\tau_c = 3.2$	446	1500	70.5	$\tau_b = 7.8$ $\tau_c = 4.8$	471
Pyrrolo[*3,4-d*]pyridazine dione -based EC Polymers (Ref.: *Org. Lett.* 2014, 16, 6386 – 6389)										
P6a	Purple	Cyan	544	34.1	$\tau_b = 7.62$ $\tau_c = 2.38$	436	1350	54.2	$\tau_b = 2.24$ $\tau_c = 7.12$	457
P6b	Purple	Cyan	530	12.4	$\tau_b = 7.47$ $\tau_c = 0.87$	282	1350	47.2	$\tau_b = 0.85$ $\tau_c = 7.35$	453
P6c	Purple	Cyan	530	10.9	$\tau_b = 8.30$ $\tau_c = 0.92$	331	1300	36.2	$\tau_b = 0.66$ $\tau_c = 8.06$	454
PPD -based EC Polymers (Ref.: *Polym. Chem.* 2015, 6, 1487 – 1494)										
P7a	Dark Blue	Sky Blue	576	11	$\tau_b = 23.2$ $\tau_c = 4.0$	205	1400	58	$\tau_b = 17.6$ $\tau_c = 23.6$	379
P7b	Dark Blue	Sky Blue	577	34	$\tau_b = 23.0$ $\tau_c = 1.8$	471	1400	71	$\tau_b = 2.59$ $\tau_c = 17.7$	651
P7c	Dark Blue	Sky Blue	574	14	$\tau_b = 25.3$ $\tau_c = 4.5$	274	1400	62	$\tau_b = 17.9$ $\tau_c = 23.6$	366
PAPD -based EC Polymers (Ref.: *Polym. Chem.* 2015, 6, 7570 – 7579)										
P8a	Dark Purple	Navy Blue	550	43.0	$\tau_b = 55.0$ $\tau_c = 10.0$	361	1500	78.6	$\tau_b = 14.5$ $\tau_c = 38.7$	353
P8b	Maroon - Purple	Grey Blue	540	32.1	$\tau_b = 50.4$ $\tau_c = 5.5$	212	1500	59.5	$\tau_b = 12.4$ $\tau_c = 29.2$	300
P8c	Dark Maroon - Purple	Dark Grey	522	16.4	$\tau_b = 73.7$ $\tau_c = 8.2$	328	1500	80.5	$\tau_b = 22.5$ $\tau_c = 31.6$	368
P8d	Dark Red	Brown Grey	510	15.5	$\tau_b = 59.8$ $\tau_c = 4.9$	239	1500	66.1	$\tau_b = 17.3$ $\tau_c = 54.8$	394
P8e	Dark Brown	Brown	505	2.0	$\tau_b = 71.5$ $\tau_c = 9.7$	156	1500	54.0	$\tau_b = 30.8$ $\tau_c = 68.6$	46.4

9. APPENDIX 1: Cartesian Coordinates from DFT Calculations

7.1. DFT calculations of free energy profiles for Diels-Alder reactions between *N*-ethyl maleimide and 3,6-bis(5-bromothiophen-2-yl)-1,2,4-triazine; and that between *N*-ethyl maleimide and 3,6-bis(5-bromothiophen-2-yl)-1,2,4,5-tetrazine.

Provided below are the Cartesian coordinates of optimized structures of reactants, transition states and intermediates. First line: total number of atoms; Second line: molecule name or comment; All other lines: element symbol or atomic number, x, y, and z coordinates, separated by spaces, tabs, or commas

N-ethyl maleimide reactant:

16

[Geometry 11]

O	0.1570030000	2.2923490000	-0.1660000000
C	0.5576420000	1.1477900000	-0.0690880000
C	1.9472110000	0.6773120000	0.2528440000
C	1.9542730000	-0.6587500000	0.2537920000
N	-0.2131870000	-0.0024310000	-0.2501960000
C	-1.6392620000	-0.0100270000	-0.5662260000
C	-2.5256480000	-0.0055340000	0.6787660000
C	0.5698070000	-1.1443200000	-0.0677050000
O	0.1812870000	-2.2931170000	-0.1634190000
H	2.7581760000	1.3701030000	0.4395800000
H	2.7724670000	-1.3427240000	0.4415730000
H	-1.8266220000	-0.9008560000	-1.1717000000
H	-1.8342440000	0.8711320000	-1.1834100000
H	-3.5812050000	-0.0120350000	0.3834940000
H	-2.3395300000	-0.8899670000	1.2974240000
H	-2.3471910000	0.8886790000	1.2854640000

Vibrational Frequencies(cm^-1)

[32.9625 108.5614 144.645 205.9101 293.9856 298.1861 346.0624
434.6653 572.0015 606.899 633.6429 703.3001 722.3374 766.5825
784.5913 835.2661 963.0932 964.9966 993.2677 1064.9117 1113.2655
1126.7881 1154.3895 1244.2545 1338.4411 1379.9801 1397.0794 1430.6122
1441.1863 1496.9493 1515.532 1524.3052 1660.3768 1787.5511 1848.2822
3058.441 3093.6434 3126.5284 3128.9487 3150.1934 3258.4933 3277.8934]

Precursor **7** (3,6-bis(5-bromothiophen-2-yl)-1,2,4-triazine):

23

[Geometry 8]

Br	-6.9359820000	-0.4296220000	0.0000220000
C	-5.1966700000	0.2939750000	-0.0000090000
C	-4.8623710000	1.6212570000	-0.0000440000
C	-3.4528410000	1.8062240000	-0.0000480000
C	-2.7405440000	0.6265840000	-0.0000170000
S	-3.8166280000	-0.7634250000	-0.0000920000
C	-1.3051770000	0.4101420000	0.0000080000
C	-0.3474960000	1.4504530000	0.0000300000
N	0.9430280000	1.1821040000	0.0000690000
C	1.2825370000	-0.1275060000	0.0001040000
C	2.6968340000	-0.4620150000	0.0000550000
C	3.2853630000	-1.7073990000	0.0000100000
C	4.7046860000	-1.6610980000	-0.0000200000
C	5.1688050000	-0.3716900000	-0.0000040000
Br	6.9710130000	0.1778440000	-0.0000260000
S	3.8990890000	0.8146630000	0.0000230000
N	0.4038490000	-1.1463310000	0.0000540000
N	-0.8875030000	-0.8693270000	0.0000190000
H	-5.5858590000	2.4278590000	-0.0000510000
H	-2.9876610000	2.7860590000	-0.0000570000
H	-0.6406310000	2.4976530000	0.0000380000
H	2.7073340000	-2.6240910000	0.0000080000
H	5.3470100000	-2.5337470000	-0.0000490000

Vibrational Frequencies(cm^-1)

[19.7208 39.7069 52.5839 63.4139 85.9944 90.1266 115.0419
165.4313 195.2006 207.3218 237.9118 260.5789 279.9015 369.3445
372.4646 380.9563 399.1611 459.1698 468.9337 488.7817 517.7804
555.9261 587.7856 622.9418 655.3334 660.412 668.5978 730.3608
737.9915 783.7551 810.9663 824.0126 841.5577 913.1092 931.9812
954.3918 961.9011 973.272 987.1751 1009.2353 1075.4834 1091.1232
1112.3945 1163.6252 1231.4854 1245.5153 1290.8159 1318.6294 1372.8588
1379.9478 1391.9555 1445.5378 1476.1027 1483.4287 1539.0069 1588.6483
1597.6379 1621.0146 3205.5794 3233.6391 3244.8074 3250.2152 3256.0439]

Transition state of IIEDA reaction of *N*-ethyl maleimide over 1,2,4-triazine moiety of precursor **7**:

39

[Geometry 11]

Br	-7.0430930000	-0.9932780000	-0.1712220000
C	-5.2530070000	-0.4661400000	-0.4395780000
S	-3.9646300000	-1.3511660000	0.3222630000
C	-4.8094570000	0.5700760000	-1.2149780000
C	-3.3906350000	0.6743460000	-1.1936640000
C	-2.7851970000	-0.2801570000	-0.4123990000
C	-1.3608340000	-0.4831080000	-0.1438200000
N	-0.4773840000	0.0824520000	-1.0850790000
N	0.7675920000	-0.0999110000	-0.8968630000
N	-1.0267350000	-1.6936840000	0.4532990000
C	0.2421380000	-1.8712020000	0.6311270000
C	1.1663590000	-0.8170880000	0.2510700000
C	2.6117350000	-1.0230460000	0.3733790000
C	3.2960430000	-1.7051560000	1.3520400000
C	4.7045920000	-1.7285880000	1.1506190000
C	5.0605040000	-1.0581510000	0.0125980000
Br	6.8052440000	-0.8330400000	-0.6656690000
S	3.7053190000	-0.3832350000	-0.8383280000
C	0.5597480000	0.5600710000	1.6580620000
C	-0.8156570000	0.7992700000	1.4377030000
C	-0.9474120000	2.1866490000	0.8782710000
N	0.3523020000	2.6749370000	0.7099940000
C	0.6704670000	3.9595190000	0.0897030000
C	0.8936300000	3.8364310000	-1.4174410000
C	1.3016580000	1.8108630000	1.2505220000
O	2.4862180000	2.0508370000	1.3778200000
O	-1.9640700000	2.8066810000	0.6311150000
H	-5.4628680000	1.2282000000	-1.7751490000
H	-2.8354530000	1.4306100000	-1.7339870000
H	0.6011580000	-2.8127560000	1.0409300000
H	2.8114400000	-2.1727880000	2.2030650000
H	5.4106470000	-2.2151520000	1.8126710000
H	0.9402160000	-0.0034350000	2.5013630000

H -1.6026890000 0.4152270000 2.0747880000
H 1.5654910000 4.3400740000 0.5884530000
H -0.1624650000 4.6324270000 0.3092620000
H 1.1256660000 4.8213260000 -1.8385390000
H 1.7279830000 3.1626040000 -1.6375730000
H -0.0011160000 3.4509690000 -1.9172660000

Vibrational Frequencies(cm^-1)
[-522.2037 20.9567 27.2529 35.5633 39.9067 47.5893 53.0207
62.2407 75.0214 87.9326 102.6068 127.32 150.79 155.7867
163.9214 177.2303 181.09 206.2595 208.936 236.3005 250.9918
281.0447 300.2721 304.1229 355.1107 370.1837 377.075 389.4406
418.4297 437.3038 456.5433 467.8538 484.8087 511.716 522.4731
531.71 583.187 589.6497 602.6215 626.0781 650.2187 665.6656
671.0204 691.3699 710.8833 726.6208 732.5352 738.017 745.4321
761.0668 777.7739 797.935 818.0309 820.1565 902.114 909.5705
912.2662 919.8233 954.8795 956.9992 969.5581 974.7922 992.4276
998.0698 1003.321 1058.1952 1066.7191 1087.0038 1094.5652 1105.7213
1110.0793 1133.2352 1135.7848 1232.3706 1248.748 1251.7829 1277.4377
1305.7213 1320.1781 1326.4328 1369.7208 1374.4552 1380.7072 1390.0405
1396.8933 1421.4809 1427.348 1441.2654 1469.7354 1481.6049 1487.8621
1497.34 1513.616 1521.4484 1595.3616 1599.6163 1639.4788 1782.4786
1842.0277 3060.953 3097.1922 3130.7487 3132.6341 3154.4216 3200.2642
3227.6383 3235.0902 3247.3103 3247.8989 3255.4092 3262.3933]

Transition state of Diels Alder reaction of *N*-ethyl maleimide over thiophene moiety of precursor **7**:

[Geometry 16]
Br 8.1416890000 -0.2615130000 -0.4342480000
C 6.3865860000 0.1676360000 0.0904210000
C 5.9872570000 1.2277890000 0.8595620000
C 4.5812850000 1.2404580000 1.0538660000
C 3.9244970000 0.1976380000 0.4360120000
S 5.0631120000 -0.8382070000 -0.4135920000
C 2.4934650000 -0.0641480000 0.4465780000
C 1.8820050000 -1.1452590000 -0.2292490000
N 0.5761850000 -1.3245670000 -0.1879580000
C -0.1184430000 -0.4224420000 0.5348320000

C	-1.5733330000	-0.5662400000	0.5914500000
C	-2.4339830000	0.1138270000	1.5048290000
C	-3.7377610000	-0.2841870000	1.3804270000
C	-3.8821920000	-1.1886220000	0.2689960000
Br	-5.4815740000	-2.2294800000	0.0840920000
S	-2.3345700000	-2.0608890000	0.0258240000
C	-3.7421450000	0.0155370000	-1.2940000000
C	-4.6331980000	1.1982130000	-0.9814100000
N	-3.7883870000	2.2730710000	-0.7122240000
C	-4.2494650000	3.6133650000	-0.3611790000
C	-4.2623400000	3.8735570000	1.1448250000
O	-5.8492090000	1.2327780000	-0.9562080000
C	-2.4170840000	0.5178610000	-1.3369000000
C	-2.4449570000	1.9564080000	-1.0012410000
O	-1.5295480000	2.7617990000	-0.9825790000
N	0.4196310000	0.6117480000	1.2019890000
N	1.7285000000	0.7884810000	1.1578000000
H	6.6689780000	1.9648810000	1.2668450000
H	4.0563520000	1.9934540000	1.6294880000
H	2.4624290000	-1.8659750000	-0.8030670000
H	-2.0777480000	0.9221840000	2.1322580000
H	-4.5866050000	0.1504020000	1.8945600000
H	-4.1181780000	-0.7001190000	-2.0174320000
H	-5.2533700000	3.7222050000	-0.7802290000
H	-3.5834740000	4.3193600000	-0.8649880000
H	-3.2594860000	3.7682610000	1.5718800000
H	-4.9390380000	3.1835590000	1.6603130000
H	-4.6080380000	4.8953860000	1.3394630000
H	-1.6050980000	0.1106200000	-1.9232190000

Vibrational Frequencies(cm^-1)

[-501.2661 17.9867 23.3737 29.9045 34.6992 45.802 53.3075
64.9749 73.0045 78.0508 100.4542 114.4262 133.0058 143.295
163.2171 170.5175 194.3489 207.5896 222.5971 235.4552 253.4939
262.8973 290.3491 308.9432 348.9041 349.8435 364.7904 389.0723
392.775 411.4406 436.7981 447.1192 457.798 485.9538 501.0069
550.804 575.2012 599.8662 610.8538 625.3008 637.1748 651.6397

663.3283 695.0507 713.9709 721.6456 734.5625 748.6594 772.1502
781.8048 791.7888 806.1769 821.9524 837.9312 862.8492 923.4533
931.9791 951.8441 957.8296 959.5838 964.9864 985.0349 998.4375
1003.6564 1039.8811 1052.2444 1079.0103 1091.1409 1109.6765 1131.4679
1134.0848 1148.3563 1154.8074 1185.2637 1217.1828 1233.7196 1245.4528
1302.3792 1322.9645 1328.9467 1371.2244 1377.7841 1390.7309 1391.3309
1395.692 1420.3297 1431.3824 1437.9118 1465.2546 1478.5431 1494.0452
1516.0211 1524.6967 1529.6162 1544.2324 1591.8358 1607.8215 1776.2162
1835.4976 3057.7023 3091.4975 3125.4953 3128.1458 3149.6927 3187.1324
3218.0261 3247.4296 3247.6418 3258.6608 3261.5932 3267.2246]

Intermediate product of IIEDA reaction of *N*-ethyl maleimide over 1,2,4-triazine moiety of precursor **7**:

39

[Geometry 47]

Br	-6.8628280000	-0.8671280000	0.7475280000
C	-5.1692070000	-0.8550420000	-0.0873910000
S	-3.7444370000	-0.5035790000	0.8446020000
C	-4.8998850000	-1.1086390000	-1.4025050000
C	-3.5033580000	-1.0120770000	-1.6794400000
C	-2.7514900000	-0.6872460000	-0.5821590000
C	-1.2695140000	-0.5158070000	-0.4847490000
N	-0.5710110000	-1.7343040000	-1.1204270000
N	0.6468340000	-1.7583400000	-0.9928950000
N	-0.8423770000	-0.3730820000	0.8873240000
C	0.4317960000	-0.4109550000	1.0162150000
C	1.2671660000	-0.5476720000	-0.2228800000
C	2.7167700000	-0.8797990000	-0.0096140000
C	3.1613810000	-2.1445990000	0.2908140000
C	4.5737700000	-2.2476790000	0.4469160000
C	5.1818220000	-1.0419080000	0.2519680000
Br	7.0300790000	-0.6681930000	0.3520630000
S	4.0644270000	0.2434790000	-0.0992830000
C	0.8665030000	0.6607810000	-1.1522910000
C	-0.6601880000	0.6432470000	-1.3577240000
C	-1.1478510000	2.0227780000	-0.9157080000
N	-0.0467110000	2.7345330000	-0.4463570000
C	-0.1440120000	4.0982360000	0.0852790000

C	-0.3912770000	4.1179550000	1.5926150000
C	1.1465040000	2.0379080000	-0.5355570000
O	2.2268790000	2.4788500000	-0.1924950000
O	-2.2790010000	2.4552770000	-0.9697150000
H	-5.6554110000	-1.3534640000	-2.1396640000
H	-3.0790760000	-1.1854310000	-2.6627290000
H	0.8911410000	-0.3753720000	2.0027440000
H	2.4917970000	-2.9935260000	0.3768290000
H	5.0999600000	-3.1649460000	0.6831890000
H	1.4198520000	0.5752920000	-2.0916140000
H	-0.9542730000	0.4772660000	-2.3964880000
H	0.7912990000	4.6035070000	-0.1659400000
H	-0.9618110000	4.5843610000	-0.4516000000
H	-0.4657680000	5.1553500000	1.9370150000
H	-1.3254440000	3.6059580000	1.8452110000
H	0.4303410000	3.6373100000	2.1337060000

Vibrational Frequencies(cm^-1)

[20.8959 23.0346 28.7016 41.0555 48.6158 55.5376 66.4386
75.307 88.203 123.1772 132.421 138.8701 156.572 176.0442
188.2962 208.8793 220.5863 235.8491 250.4647 280.0972 307.7985
318.6008 340.4495 354.6552 366.2611 375.2107 391.9682 412.7532
444.4783 466.0685 489.5414 508.6745 516.7952 522.3441 572.7801
575.1061 589.9401 605.1876 611.0844 643.1338 649.8876 668.5796
684.9141 708.14 733.1082 734.3339 742.0088 759.3278 792.411
801.3703 810.3107 819.9426 830.7722 878.7284 893.7695 902.1694
906.8958 938.6036 947.8157 957.124 964.4025 973.1873 984.3542
1018.3838 1030.5892 1047.3516 1083.6871 1085.2697 1091.774 1126.0363
1132.3803 1162.4468 1213.5523 1246.1768 1255.2616 1264.8708 1269.8939
1276.8869 1297.7083 1307.0626 1323.5837 1355.252 1362.0392 1370.374
1389.3444 1394.9848 1423.7998 1441.254 1490.9862 1494.4655 1497.1389
1515.8699 1523.726 1591.0556 1605.7974 1623.8226 1708.4242 1784.6473
1855.4492 3062.9556 3104.5688 3116.4104 3132.1286 3133.8342 3135.93
3161.8003 3193.3208 3229.4536 3233.193 3249.5466 3251.1956]

Intermediate product of Diels-Alder reaction of *N*-ethyl maleimide over thiophene moiety of precursor **7**:

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[Geometry 2]

Br	8.1500270000	-0.0577650000	-0.4923100000
C	6.4113450000	-0.0267160000	0.2264560000
C	6.0608880000	0.1219840000	1.5415950000
C	4.6525120000	0.0982620000	1.7192710000
C	3.9467090000	-0.0664310000	0.5473570000
S	5.0385810000	-0.1990450000	-0.8234280000
C	2.4991100000	-0.1331150000	0.3989490000
C	1.8389870000	-0.2770540000	-0.8438290000
N	0.5232600000	-0.3335990000	-0.9138320000
C	-0.1323840000	-0.2454020000	0.2590020000
C	-1.6321280000	-0.3298250000	0.2247300000
C	-2.3893190000	-0.0134420000	1.5092070000
C	-3.6457520000	-0.4587460000	1.4334010000
C	-3.8660170000	-1.1316340000	0.0902640000
Br	-5.4508870000	-2.2571090000	-0.0250130000
S	-2.2785810000	-2.0616940000	-0.1889520000
C	-3.7759000000	-0.0377290000	-1.0234450000
C	-4.6572040000	1.1901610000	-0.7901560000
N	-3.8219080000	2.2907680000	-0.6035990000
C	-4.3276170000	3.6400090000	-0.3375500000
C	-4.5390500000	3.9041970000	1.1526070000
O	-5.8704960000	1.2342620000	-0.7756150000
C	-2.3245510000	0.4889110000	-0.9325540000
C	-2.4651890000	1.9802040000	-0.6379810000
O	-1.5665830000	2.7809730000	-0.4658980000
N	0.4470570000	-0.1099900000	1.4543110000
N	1.7716380000	-0.0519430000	1.5264870000
H	6.7782040000	0.2429080000	2.3445630000
H	4.1615190000	0.1996780000	2.6797380000
H	2.3889310000	-0.3434750000	-1.7812980000
H	-1.9544050000	0.5831240000	2.3018240000
H	-4.4486940000	-0.2932620000	2.1421580000
H	-4.0143890000	-0.4758360000	-1.9945520000
H	-5.2666490000	3.7389240000	-0.8873920000
H	-3.5994220000	4.3379290000	-0.7575820000
H	-3.5999330000	3.8067390000	1.7070540000

H -5.2709890000 3.2084000000 1.5756110000
H -4.9154730000 4.9233280000 1.2953460000
H -1.7589410000 0.3536450000 -1.8564810000

Vibrational Frequencies(cm^-1)
[15.2017 27.2838 34.4374 42.6068 55.1338 59.0318 61.4242
66.893 95.9456 101.5395 118.0319 132.8026 145.4811 176.3516
202.4465 212.3271 224.6703 231.8499 258.947 265.3905 298.5235
314.7907 319.024 357.7747 365.9412 373.8235 397.5635 408.5428
417.7512 430.2538 459.271 478.4494 488.4908 544.0961 555.1766
590.2833 601.2454 609.4803 619.7133 653.4995 664.5795 667.7625
683.6188 714.7557 734.5938 740.2258 770.1689 783.2986 800.0202
819.5978 835.1288 840.9027 870.0159 912.7443 930.9802 934.9045
946.641 957.0791 958.5707 969.8945 988.5436 1000.286 1024.3765
1032.147 1058.0707 1084.8702 1085.5644 1092.4423 1092.902 1126.4935
1140.1609 1155.8545 1160.9506 1231.6908 1246.2234 1260.2734 1265.0317
1285.1302 1301.2943 1310.4267 1315.5339 1336.1512 1372.845 1387.7732
1390.7162 1391.8207 1420.2363 1438.969 1450.1703 1476.2875 1498.1421
1515.7694 1525.2091 1539.1097 1593.0964 1611.848 1663.2726 1786.8974
1852.6575 3062.0934 3101.3374 3131.773 3132.8363 3133.4337 3139.9645
3158.5306 3180.5134 3243.3371 3247.993 3258.8535 3263.0281]

3,6-bis(5-bromothiophen-2-yl)-1,2,4,5-tetrazine:
22
[Geometry 6]
Br 6.9342140000 0.2924420000 0.0000760000
C 5.1585750000 -0.3246950000 0.0000140000
C 4.7454300000 -1.6385230000 -0.0000230000
C 3.3306160000 -1.7447590000 -0.0000560000
C 2.6928190000 -0.5184800000 -0.0000450000
S 3.8389220000 0.8027640000 -0.0000800000
C 1.2675870000 -0.2500440000 -0.0000480000
N 0.4115520000 -1.2939340000 -0.0000380000
N -0.8643830000 -1.0389970000 -0.0000320000
C -1.2675870000 0.2500460000 -0.0000280000
C -2.6928190000 0.5184810000 -0.0000320000
C -3.3306170000 1.7447600000 -0.0000500000

C -4.7454310000 1.6385230000 -0.0000160000
C -5.1585750000 0.3246940000 0.0000120000
Br -6.9342130000 -0.2924430000 0.0000680000
S -3.8389210000 -0.8027640000 -0.0000600000
N -0.4115530000 1.2939360000 -0.0000360000
N 0.8643840000 1.0389990000 -0.0000440000
H 5.4279980000 -2.4886590000 -0.0000080000
H 2.7842370000 -2.6884610000 -0.0000670000
H -2.7842390000 2.6884620000 -0.0000600000
H -5.4280000000 2.4886580000 -0.0000010000

Vibrational Frequencies(cm^-1)
[14.3717 37.1232 47.2376 61.965 84.1208 91.2662 104.5349
164.3863 194.5339 208.2639 234.3046 256.2842 280.9496 375.3313
377.2952 383.3467 385.3193 465.7583 471.7477 486.3246 530.6314
564.7882 601.1305 661.9332 665.5288 674.2124 677.2455 736.8865
742.869 802.0511 826.1562 836.3269 863.6116 942.822 944.6225
969.4549 970.1485 1006.3539 1018.9564 1066.7768 1075.8336 1084.4481
1114.0904 1210.3308 1215.2101 1308.0898 1310.6989 1387.8049 1394.8925
1437.4851 1474.6828 1482.8058 1510.7517 1545.4879 1591.5768 1598.2664
3226.7736 3226.7818 3237.5861 3237.5912]

Transition state of IIEDA reaction of *N*-ethyl maleimide over tetrazine moiety of 3,6-bis(5-bromothiophen-2-yl)-1,2,4,5-tetrazine:

38
[Geometry 7]
Br -7.0150490000 -1.0150470000 -0.0830800000
C -5.2432980000 -0.4813120000 -0.4211040000
S -3.9199400000 -1.3089970000 0.3417570000
C -4.8318040000 0.5268290000 -1.2597290000
C -3.4153440000 0.6513820000 -1.2814240000
C -2.7775850000 -0.2604030000 -0.4688700000
C -1.3432350000 -0.4248590000 -0.2364240000
N -0.4788750000 0.1358300000 -1.1786530000
N 0.7622100000 -0.0536040000 -0.9948840000
N -0.9587530000 -1.6457170000 0.3345160000
N 0.2779170000 -1.8403080000 0.5102820000
C 1.1384420000 -0.8028180000 0.1205960000

C	2.5721830000	-1.0601790000	0.2682820000
C	3.1908330000	-1.9203810000	1.1507340000
C	4.6045830000	-1.9486770000	1.0070220000
C	5.0311710000	-1.1074400000	0.0057190000
Br	6.8077520000	-0.8233970000	-0.5450950000
S	3.7281150000	-0.2746070000	-0.7790040000
C	0.5525130000	0.5321590000	1.6171040000
C	-0.8171710000	0.7669450000	1.4022320000
C	-0.9568960000	2.1737370000	0.8715520000
N	0.3386330000	2.6705070000	0.7263830000
C	0.6570030000	3.9735740000	0.1517710000
C	0.9408560000	3.9053370000	-1.3464330000
C	1.2914350000	1.7949680000	1.2476930000
O	2.4675130000	2.0338120000	1.3863120000
O	-1.9745390000	2.7809050000	0.6329530000
H	-5.5132750000	1.1520100000	-1.8370640000
H	-2.8784030000	1.3889610000	-1.8772290000
H	2.6404250000	-2.5214730000	1.8757300000
H	5.2735920000	-2.5637890000	1.6092130000
H	0.9460790000	-0.0996780000	2.4134670000
H	-1.6132270000	0.3506280000	2.0194520000
H	1.5300590000	4.3606910000	0.6972980000
H	-0.1991180000	4.6316330000	0.3598110000
H	1.1758600000	4.9122360000	-1.7268600000
H	1.7992410000	3.2498920000	-1.5603020000
H	0.0695400000	3.5242210000	-1.9014240000

Vibrational Frequencies(cm^-1)

[-523.5238 17.7725 24.547 30.6973 41.6742 50.3422 56.5529
60.3687 71.0244 88.7702 101.7647 126.1632 149.2057 157.8042
166.3758 178.211 184.3501 204.7529 211.6337 238.9683 250.6021
281.4323 298.639 309.9372 361.5032 374.516 383.6202 388.3445
426.299 431.3666 462.523 472.3104 486.5922 529.4625 534.0253
535.3615 592.1258 593.6749 605.5429 626.9887 658.6134 671.2448
692.3347 703.1123 714.1537 737.3249 738.5109 743.386 747.9686
771.4097 781.354 794.8539 823.8745 827.3318 921.0671 925.8108
930.3837 957.2063 963.4448 972.5008 991.186 992.1899 1003.3278

1006.405 1032.0059 1058.5394 1071.9323 1074.5293 1082.7151 1098.3605
1120.9969 1127.5166 1210.1881 1217.759 1237.1039 1269.4595 1303.0169
1320.8473 1330.4087 1369.5365 1374.4055 1376.8056 1394.4725 1400.3354
1416.6031 1421.3147 1447.6336 1457.6486 1463.6002 1469.3833 1476.646
1480.8024 1583.1533 1595.7348 1607.0825 1806.7574 1865.6251 3040.7177
3077.9145 3124.2106 3127.5579 3143.4254 3217.9763 3220.4387 3227.8146
3228.5739 3233.0722 3241.5315]

Calculations for Diels Alder reaction of *N*-ethyl maleimide over thiophene moiety of 3,6-bis(5-bromothiophen-2-yl)-1,2,4,5-tetrazine:

38

[Geometry 10]

Br	7.9984290000	-0.3611660000	-0.5536120000
C	6.2921660000	0.1371150000	0.0548860000
C	5.9887400000	1.2175660000	0.8549000000
C	4.5990400000	1.2983070000	1.1227810000
C	3.8706250000	0.2847970000	0.5267190000
S	4.8986510000	-0.7977050000	-0.3847580000
C	2.4413590000	0.0605090000	0.5853730000
N	1.9353910000	-0.9994040000	-0.0812380000
N	0.6476230000	-1.1892120000	-0.0514920000
C	-0.1075520000	-0.3219020000	0.6460990000
C	-1.5574000000	-0.5122970000	0.6417190000
C	-2.4662760000	0.1505760000	1.5266860000
C	-3.7528070000	-0.2874950000	1.3590650000
C	-3.8305880000	-1.2247010000	0.2652000000
Br	-5.3850630000	-2.3136680000	0.0358770000
S	-2.2479030000	-2.0468620000	0.0905780000
C	-3.6325730000	-0.0075150000	-1.3169370000
C	-4.5443260000	1.1734910000	-1.0710540000
N	-3.7197440000	2.2566290000	-0.7604740000
C	-4.2094610000	3.5947490000	-0.4541410000
C	-4.3542960000	3.8723630000	1.0398330000
O	-5.7529110000	1.2091220000	-1.1252850000
C	-2.3070630000	0.4986800000	-1.2832180000
C	-2.3636520000	1.9470990000	-0.9657750000
O	-1.4550090000	2.7482810000	-0.8989190000
N	0.3970910000	0.7155430000	1.3435530000

N 1.6833200000 0.9098770000 1.3152190000
H 6.7316080000 1.9207410000 1.2320210000
H 4.1330260000 2.0730560000 1.7324910000
H -2.1531550000 0.9791330000 2.1626350000
H -4.6353360000 0.1312190000 1.8438130000
H -3.9628110000 -0.7439150000 -2.0515410000
H -5.1799390000 3.7036360000 -0.9606980000
H -3.5015280000 4.3049380000 -0.9068640000
H -3.3881210000 3.7804490000 1.5602410000
H -5.0744810000 3.1836470000 1.5089110000
H -4.7227270000 4.8996270000 1.1925510000
H -1.4643350000 0.0984440000 -1.8441230000

Vibrational Frequencies(cm^-1)

[-521.9507 13.8511 22.3892 24.6782 35.2388 49.2565 59.9381
70.5941 77.486 86.2074 97.9738 111.7328 138.8895 148.6475
166.3396 175.7112 195.3804 207.8915 227.5065 232.3249 250.0286
265.6791 291.1985 314.076 356.3132 358.0653 376.4527 380.3412
394.7259 418.7567 440.4672 455.7939 464.7688 491.77 509.5036
560.5513 581.1458 603.4432 627.7252 644.3937 651.4961 668.844
675.3572 695.8654 717.2321 731.0829 739.7872 762.9629 778.1475
791.7397 799.6848 804.5689 830.318 860.6261 886.4027 927.5351
944.8861 963.2701 965.1145 970.2224 990.4801 1000.8803 1014.961
1022.6069 1037.8492 1071.7024 1078.7527 1100.2799 1100.4114 1123.4924
1125.9391 1144.2527 1165.166 1206.4164 1217.1806 1232.3908 1309.9849
1311.5392 1367.4572 1374.5564 1377.6619 1384.0551 1393.2023 1398.1883
1416.5109 1420.6036 1443.9486 1459.915 1466.8752 1471.761 1489.7988
1516.0427 1537.6634 1552.2025 1594.1535 1796.884 1856.2846 3037.4057
3070.9576 3118.7662 3122.1507 3137.951 3205.3705 3225.5993 3226.1212
3236.5881 3240.8759 3244.5585]

Intermediate formed for IIEDA reaction of *N*-ethyl maleimide over tetrazine moiety of 3,6-bis(5-bromothiophen-2-yl)-1,2,4,5-tetrazine:

38

[Geometry 19]

Br 6.9312580000 -1.2772960000 0.1511500000
C 5.1745160000 -0.6694470000 0.4541150000
S 3.8763280000 -1.1945300000 -0.5755090000

C	4.7495090000	0.1663690000	1.4551480000
C	3.3451950000	0.4070900000	1.3857150000
C	2.7342060000	-0.2439110000	0.3433380000
C	1.2928370000	-0.2086330000	-0.0490620000
N	0.4274660000	0.0362830000	1.1249630000
N	-0.7845370000	-0.0980450000	0.9151150000
N	0.8928580000	-1.5031350000	-0.6770920000
N	-0.3132240000	-1.6420230000	-0.8799640000
C	-1.1568960000	-0.4755540000	-0.4616550000
C	-2.6109510000	-0.8047070000	-0.5452920000
C	-3.2851170000	-1.3830570000	-1.5920120000
C	-4.6737960000	-1.5759050000	-1.3299110000
C	-5.0183980000	-1.1398470000	-0.0751930000
Br	-6.7293170000	-1.1924760000	0.7121250000
S	-3.6683800000	-0.4964840000	0.8081080000
C	-0.6373550000	0.6971560000	-1.3780330000
C	0.8585480000	0.8685590000	-1.1207650000
C	1.0186990000	2.3134170000	-0.6324790000
N	-0.2456450000	2.8922520000	-0.5958810000
C	-0.4798050000	4.2705370000	-0.1648100000
C	-0.7768920000	4.3805420000	1.3277820000
C	-1.2647960000	2.0523400000	-1.0322930000
O	-2.4255980000	2.3634710000	-1.1363750000
O	2.0479310000	2.8768110000	-0.3508550000
H	5.4088210000	0.5908360000	2.2126340000
H	2.8054610000	1.0453170000	2.0850970000
H	-2.8030760000	-1.6747420000	-2.5265990000
H	-5.3776890000	-2.0184850000	-2.0351640000
H	-0.8819570000	0.4385450000	-2.4171160000
H	1.4818910000	0.7163060000	-2.0124060000
H	-1.3223950000	4.6515090000	-0.7592100000
H	0.4211330000	4.8428320000	-0.4275240000
H	-0.9463590000	5.4359510000	1.5937520000
H	-1.6802430000	3.8123390000	1.5986990000
H	0.0651890000	4.0085750000	1.9319350000

Vibrational Frequencies(cm^-1)

[15.8529 22.4602 31.6069 37.2911 41.4507 59.0841 62.8609
68.3265 89.8217 120.4783 130.4734 150.9974 162.7977 170.6883
194.1154 204.2332 227.4536 242.9472 247.9458 287.5397 307.2407
317.9635 339.6388 364.3522 376.2405 382.4258 399.5891 440.4631
445.8682 479.5375 483.6697 522.8812 534.6521 535.2654 583.6266
589.376 593.2878 605.5903 643.4943 658.0414 669.3974 703.3602
714.0631 731.8182 740.7182 742.6786 750.1293 752.2564 800.8867
811.8433 821.8338 825.2068 858.6545 876.1807 893.4123 904.8917
915.2365 925.7174 964.6884 966.4421 975.3458 977.799 1005.8498
1018.8448 1052.5061 1057.8218 1068.7 1073.8601 1088.8909 1113.9853
1144.9491 1215.9989 1220.4934 1224.988 1249.5219 1252.2064 1257.0366
1290.1987 1295.5315 1309.4723 1354.7127 1357.9211 1376.7779 1382.3332
1398.7111 1417.6276 1447.183 1458.564 1470.9137 1492.9729 1495.1194
1584.9709 1602.1883 1612.5278 1713.7071 1814.2769 1879.1063 3041.6096
3083.1532 3115.8539 3121.6431 3126.5523 3129.3521 3148.3899 3214.4603
3225.3184 3231.1739 3237.2734]

Calculations for Diels-Alder reaction of *N*-ethyl maleimide over thiophene moiety of 3,6-bis(5-bromothiophen-2-yl)-1,2,4,5-tetrazine:

38

[Geometry 8]

Br	-7.7139820000	0.4652080000	-0.7820600000
C	-6.1130570000	-0.1231420000	0.0067830000
C	-5.9830280000	-0.7694550000	1.2166780000
C	-4.6280340000	-1.0705810000	1.5075340000
C	-3.7547080000	-0.6516070000	0.5214950000
S	-4.5968620000	0.1292750000	-0.7968770000
C	-2.3116150000	-0.7894240000	0.4881050000
N	-1.6533350000	-0.3096190000	-0.5877160000
N	-0.3524490000	-0.3993620000	-0.6041420000
C	0.2554820000	-0.9654320000	0.4462330000
C	1.7520930000	-1.0255340000	0.4565280000
C	2.3840890000	-2.3775090000	0.7802520000
C	3.6709450000	-2.3753140000	0.4217630000
C	4.0344380000	-1.0207100000	-0.1688100000
Br	5.6873210000	-1.0184800000	-1.1915040000
S	2.5295560000	-0.5806240000	-1.1832860000
C	3.9570320000	-0.0053800000	1.0228610000

C	4.2570670000	1.4606030000	0.6914240000
N	3.0837650000	2.1958800000	0.8561770000
C	2.9961440000	3.6284290000	0.5800200000
C	2.6298510000	3.9308990000	-0.8705620000
O	5.3204600000	1.9339000000	0.3725050000
C	2.4634650000	-0.0097690000	1.4322990000
C	1.9984840000	1.4315540000	1.2528080000
O	0.8764970000	1.8512270000	1.4317270000
N	-0.3953670000	-1.4932020000	1.4929430000
N	-1.6979650000	-1.4072930000	1.5197600000
H	-6.8232720000	-1.0158450000	1.8660810000
H	-4.2905170000	-1.5795670000	2.4110140000
H	1.8437720000	-3.1598560000	1.3157330000
H	4.4089080000	-3.1593440000	0.5980700000
H	4.6375470000	-0.3276490000	1.8246460000
H	3.9739400000	4.0621230000	0.8339140000
H	2.2422490000	4.0407330000	1.2658330000
H	2.5765680000	5.0210190000	-1.0206080000
H	1.6505440000	3.5015020000	-1.1322240000
H	3.3834840000	3.5277950000	-1.5645900000
H	2.2867060000	-0.3164070000	2.4740020000

Vibrational Frequencies(cm^-1)

[9.149 22.4207 27.2231 35.8385 46.7266 52.3906 63.5582
82.4635 89.0277 111.9134 120.18 141.5578 145.0762 177.7918
203.9825 206.6455 221.764 235.1819 256.2185 279.6336 311.2338
316.9129 327.3424 359.0311 371.9127 378.3705 403.3827 425.1956
431.1975 443.177 461.4279 479.3781 512.8436 544.4477 571.5437
585.1219 610.0605 618.5008 643.5916 662.0913 668.4531 678.9704
698.5402 710.985 740.4954 755.6465 775.648 791.3736 806.938
824.1938 831.4999 862.5813 873.2579 930.4172 946.1675 955.1008
968.6129 971.6147 984.1774 995.6608 1003.6896 1016.7779 1028.3153
1057.1791 1064.3706 1075.6939 1083.7293 1090.0441 1104.392 1115.696
1135.8444 1150.07 1211.987 1225.9816 1237.1623 1253.3794 1257.6904
1298.6936 1302.994 1313.7928 1371.7421 1375.1974 1382.9686 1387.4084
1399.5423 1421.9216 1445.1517 1448.6448 1457.3721 1469.9072 1478.6097
1527.4357 1546.9162 1596.1978 1664.0371 1804.6469 1872.3251 3041.3937

3080.3781 3098.4928 3103.7666 3126.4113 3127.9972 3146.1934 3216.7784
3227.4234 3237.4944 3238.2024]

7.2. DFT calculations of optimized structures of structural analogues of PPyD electron acceptor:

Calculations for Phthalimide

22

[Geometry 9]

O	-0.9748280000	-2.2965080000	-0.2468740000
C	-0.5472680000	-1.1666030000	-0.1969800000
N	-1.3237790000	0.0000060000	-0.2788550000
C	-2.7731650000	0.0000100000	-0.4181600000
C	-3.5086500000	-0.0000130000	0.9217660000
C	-0.5472570000	1.1666120000	-0.1970220000
C	0.8673900000	0.6991280000	-0.0471010000
C	2.0459610000	1.4253060000	0.0748050000
C	3.2417650000	0.7013690000	0.1999940000
C	3.2417620000	-0.7013830000	0.1999800000
C	2.0459560000	-1.4253130000	0.0747770000
C	0.8673860000	-0.6991280000	-0.0471070000
O	-0.9748150000	2.2965190000	-0.2468690000
H	-3.0391480000	-0.8930060000	-1.0030710000
H	-3.0391420000	0.8930480000	-1.0030390000
H	-3.2547960000	-0.8948100000	1.5107070000
H	-4.5973870000	-0.0000090000	0.7544010000
H	-3.2547940000	0.8947610000	1.5107400000
H	2.0334860000	2.5174280000	0.0722910000
H	4.1893190000	1.2367880000	0.2989740000
H	4.1893130000	-1.2368080000	0.2989560000
H	2.0334750000	-2.5174350000	0.0722580000

Vibrational Frequencies(cm^-1)

[27.8484 74.2638 139.5037 152.9421 198.8816 202.5509 249.4037
305.5177 349.049 386.8933 429.6568 477.2969 517.9143 536.8808
611.2513 692.3158 707.3127 717.684 739.367 779.997 812.7289
814.6062 893.472 909.1267 921.4708 996.8759 1025.8475 1035.5927
1042.5512 1054.9047 1095.3129 1105.2902 1166.5007 1186.1663 1223.2604

1227.7175 1297.1269 1369.8648 1378.9977 1400.1876 1405.84 1425.901
1453.8712 1465.9747 1477.9175 1496.5734 1498.1217 1664.0704 1667.6988
1820.5991 1868.5513 3037.6571 3069.282 3119.0396 3123.8824 3138.3361
3181.9645 3194.1159 3204.5693 3207.8959]

Calculations for PPyD:

21

[Geometry 9]

O	0.9650450000	-2.2937180000	-0.2470640000
C	0.5358150000	-1.1661640000	-0.1966530000
N	1.3133390000	0.0038490000	-0.2801850000
C	2.7640220000	-0.0003630000	-0.4211020000
C	3.4997170000	0.0028990000	0.9184090000
C	0.5438710000	1.1707430000	-0.1980140000
C	-0.8756810000	0.7013520000	-0.0455720000
C	-2.0670800000	1.3985550000	0.0792680000
C	-3.2280360000	0.6130080000	0.2034150000
N	-3.2379630000	-0.7236270000	0.2050870000
C	-2.0782250000	-1.3827780000	0.0817870000
C	-0.8757320000	-0.6942890000	-0.0448570000
O	0.9654160000	2.3016510000	-0.2477940000
H	3.0255580000	-0.8965860000	-1.0027920000
H	3.0311150000	0.8892530000	-1.0105130000
H	3.2446140000	-0.8890650000	1.5109850000
H	4.5880070000	-0.0008010000	0.7492440000
H	3.2496880000	0.9007270000	1.5043040000
H	-2.1058040000	2.4896490000	0.0816160000
H	-4.2039790000	1.1015290000	0.3071450000
H	-2.1125420000	-2.4774960000	0.0844750000

Vibrational Frequencies(cm^-1)

[29.3424 74.3186 138.82 153.1031 199.8459 202.628 248.3632
305.586 347.93 377.9215 407.6744 487.6124 519.3727 541.913
616.7223 706.0272 708.0221 743.9761 758.2329 782.4444 818.536
879.6423 893.8608 910.661 973.0703 1013.4235 1033.651 1048.2413
1058.0302 1105.6191 1157.5667 1203.4631 1225.5981 1229.67 1315.8352
1349.6228 1370.143 1379.6257 1400.7912 1419.9811 1451.633 1460.2175

1466.2834 1477.8673 1500.3729 1649.4685 1666.443 1825.3468 1873.2278
3038.8167 3071.2224 3120.6637 3125.7653 3139.7546 3158.4393 3175.1688
3211.0983]

Calculations for Pyrrolopyridazine dione:

20

[Geometry 8]

O	0.9557970000	2.2987080000	-0.2479110000
C	0.5359410000	1.1691290000	-0.1981480000
N	1.3072730000	0.0000040000	-0.2822860000
C	2.7596640000	0.0000060000	-0.4234460000
C	3.4944190000	-0.0000080000	0.9161880000
C	0.5359450000	-1.1691240000	-0.1981510000
C	-0.8807280000	-0.6928160000	-0.0439370000
C	-2.0987780000	-1.3521030000	0.0857840000
N	-3.2421670000	-0.6620610000	0.2097960000
N	-3.2421700000	0.6620530000	0.2097970000
C	-2.0987830000	1.3520990000	0.0857850000
C	-0.8807300000	0.6928160000	-0.0439360000
O	0.9558050000	-2.2987010000	-0.2479150000
H	3.0227970000	0.8926820000	-1.0097120000
H	3.0227990000	-0.8926560000	-1.0097310000
H	3.2428630000	-0.8950480000	1.5055600000
H	3.2428630000	0.8950200000	1.5055790000
H	4.5823820000	-0.0000060000	0.7459090000
H	-2.1843830000	-2.4424060000	0.0935090000
H	-2.1843910000	2.4424010000	0.0935130000

Vibrational Frequencies(cm^-1)

[30.4925 73.8378 134.4174 152.9829 195.7649 201.6706 244.3519
305.1171 345.9423 370.6381 407.5028 458.4809 522.0024 545.1332
620.1412 715.1222 729.9002 758.5717 763.3793 785.8018 819.6757
904.3718 909.2248 948.7354 974.145 1031.2793 1058.8986 1074.3132
1106.0302 1161.0868 1183.7557 1227.147 1257.0773 1275.0254 1359.7165
1375.9185 1379.4268 1399.8068 1417.7281 1453.5903 1466.6063 1477.6398
1491.2391 1641.4997 1643.5739 1830.0659 1878.3916 3040.0524 3073.2075
3122.2617 3127.7482 3141.2293 3197.2806 3198.4404]

7.3. DFT calculations for optimized structures of 3 repeating units of **P1** – **P5**.

Calculations for **P1**:

122

[Geometry 42]

O	3.8570500000	-2.1496400000	0.5335270000
C	2.7327550000	-1.7023060000	0.6037220000
N	1.5832540000	-2.4919160000	0.6984320000
C	1.5996260000	-3.9486370000	0.7317690000
C	1.6846060000	-4.5175030000	2.1475940000
C	0.4208820000	-1.7272820000	0.7521520000
C	0.8610420000	-0.2927190000	0.7024700000
C	0.1172350000	0.8943330000	0.7588840000
C	-1.3256880000	1.0873470000	0.8993860000
C	-1.9325930000	2.2618510000	1.3399730000
C	-3.3405800000	2.2320490000	1.3113380000
C	-3.8491770000	1.0303390000	0.8359950000
C	-5.2310990000	0.6372800000	0.6730410000
C	-5.7539050000	-0.6122180000	0.3723110000
C	-7.1643890000	-0.6319350000	0.2922030000
C	-7.7534870000	0.6019410000	0.5297670000
C	-9.1551020000	0.9552600000	0.5360940000
C	-9.7367920000	2.1795330000	0.8451870000
C	-11.1391510000	2.1618530000	0.7479660000
C	-11.6661460000	0.9306760000	0.3640950000
C	-13.1030260000	0.7010900000	0.2101860000
C	-13.7837480000	-0.4694960000	-0.1731740000
C	-15.1929640000	-0.4978580000	-0.2495390000
C	-15.5957890000	-1.8842000000	-0.6631680000
N	-14.4133460000	-2.6077650000	-0.7955480000
C	-14.3574830000	-4.0041390000	-1.2084350000
C	-14.2697110000	-4.1818890000	-2.7238000000
C	-13.2832010000	-1.8301190000	-0.5279560000
O	-12.1462920000	-2.2463830000	-0.5863800000
O	-16.7017520000	-2.3365370000	-0.8613910000
C	-15.9712800000	0.6254800000	0.0610910000
C	-17.4262900000	0.7769100000	0.0823640000

C	-18.1141240000	1.7614640000	0.7868690000
C	-19.5094110000	1.7514230000	0.5816100000
C	-19.9210040000	0.7613750000	-0.2981290000
C	-21.2656850000	0.4433180000	-0.7405280000
C	-21.7281830000	-0.6994550000	-1.3702510000
C	-23.1214840000	-0.6610140000	-1.6565050000
C	-23.7159040000	0.5065550000	-1.2452400000
S	-22.5781640000	1.5802940000	-0.5101510000
S	-18.5620320000	-0.1782140000	-0.8502930000
C	-15.1727040000	1.7658400000	0.4028370000
N	-13.8645960000	1.7988600000	0.4754840000
S	-10.3698740000	-0.2253730000	0.1164930000
S	-6.5225170000	1.8062980000	0.8488130000
S	-2.5577900000	-0.0769830000	0.4520750000
C	0.9446840000	2.0615310000	0.6632220000
N	2.2516980000	2.0767790000	0.5730240000
C	2.9836270000	0.9277890000	0.5512220000
C	4.4266260000	1.1510210000	0.4640610000
C	4.9878470000	2.4252440000	0.4119310000
C	6.3915140000	2.4303750000	0.3363640000
C	6.9401190000	1.1528690000	0.3286580000
C	8.3331760000	0.7731610000	0.2616860000
C	8.8975570000	-0.4931950000	0.3214060000
C	10.3074610000	-0.4911360000	0.2285720000
C	10.8543820000	0.7769220000	0.0955290000
C	12.2436010000	1.1611220000	-0.0226280000
C	12.7981470000	2.4331390000	0.0282610000
C	14.1996520000	2.4297790000	-0.1173080000
C	14.7555640000	1.1620030000	-0.2723310000
C	16.1726000000	0.8956110000	-0.5229610000
C	16.9143160000	-0.2744840000	-0.3106810000
C	16.4958080000	-1.6146530000	0.2212360000
N	17.6485120000	-2.3939510000	0.2584950000
C	17.6817560000	-3.7737840000	0.7256250000
C	17.9582810000	-3.8955850000	2.2236590000
C	18.7713160000	-1.7036430000	-0.2087070000
O	19.8803810000	-2.1859200000	-0.2775970000

O	15.3960760000	-2.0001180000	0.5524100000
C	18.2998340000	-0.3343950000	-0.5751730000
C	18.9898460000	0.7839550000	-1.0768800000
C	20.4128940000	0.9306970000	-1.4015160000
C	20.9489710000	2.1139550000	-1.8996560000
C	22.3408900000	2.0512140000	-2.1441620000
C	22.8650010000	0.8175320000	-1.8314790000
S	21.6761890000	-0.2773520000	-1.2399130000
N	18.2560690000	1.9061490000	-1.3110320000
C	16.9695910000	1.9562740000	-1.0631040000
S	13.4865570000	-0.0456570000	-0.2226590000
S	9.5858840000	1.9833190000	0.0769700000
S	5.6916930000	-0.0636660000	0.4116830000
C	2.2693050000	-0.2835260000	0.6069420000
O	-0.6987900000	-2.1858080000	0.8122420000
H	0.6804700000	-4.2898240000	0.2332200000
H	2.4641770000	-4.2712040000	0.1334670000
H	1.6933170000	-5.6182480000	2.1101180000
H	2.6059080000	-4.1867830000	2.6511820000
H	0.8191460000	-4.2044670000	2.7515580000
H	-1.3702160000	3.1214970000	1.7037010000
H	-3.9699780000	3.0575580000	1.6469980000
H	-5.1286710000	-1.4946130000	0.2271760000
H	-7.7438320000	-1.5303780000	0.0742030000
H	-9.1608460000	3.0591170000	1.1375220000
H	-11.7884560000	3.0118750000	0.9479610000
H	-15.2621060000	-4.4899110000	-0.8143900000
H	-13.4791230000	-4.4465650000	-0.7162800000
H	-14.2303150000	-5.2536730000	-2.9745130000
H	-13.3623920000	-3.7050150000	-3.1251800000
H	-15.1490590000	-3.7476210000	-3.2237140000
H	-17.6232980000	2.4604650000	1.4639430000
H	-20.2002770000	2.4323700000	1.0808590000
H	-21.0827050000	-1.5480150000	-1.6031100000
H	-23.6645270000	-1.4718500000	-2.1442290000
H	-24.7610080000	0.7997540000	-1.3342580000
H	-15.6789440000	2.7155050000	0.6052630000

H 0.4615260000 3.0437950000 0.6393950000
H 4.3616470000 3.3149690000 0.4317790000
H 6.9925500000 3.3401510000 0.2929220000
H 8.3019940000 -1.3998610000 0.4386880000
H 10.9165530000 -1.3954410000 0.2713320000
H 12.2085090000 3.3373950000 0.1861600000
H 14.7972950000 3.3404570000 -0.0823300000
H 18.4624460000 -4.2878630000 0.1461800000
H 16.7076200000 -4.2189270000 0.4752620000
H 18.9352720000 -3.4586440000 2.4811580000
H 17.1777460000 -3.3890540000 2.8119010000
H 17.9716310000 -4.9568590000 2.5180340000
H 20.3217480000 2.9863840000 -2.0725350000
H 22.9316630000 2.8809960000 -2.5349030000
H 23.9004170000 0.4883890000 -1.9193950000
H 16.4779730000 2.8999500000 -1.3216790000

Vibrational Frequencies(cm^-1)

[1.6837000e+00 3.0722000e+00 4.3373000e+00 5.0582000e+00 6.1892000e+00
9.7411000e+00 1.3175700e+01 1.4293300e+01 1.7146000e+01 1.9492900e+01
2.2344200e+01 2.5234500e+01 2.6228800e+01 2.7066200e+01 2.8073300e+01
3.1278900e+01 3.5101200e+01 3.9639200e+01 4.0823700e+01 4.2950200e+01
4.4846100e+01 4.6359700e+01 4.6497200e+01 4.6967300e+01 4.9330600e+01
5.2244200e+01 5.3373100e+01 6.0915900e+01 7.4232300e+01 7.5982000e+01
7.8953900e+01 8.0776000e+01 8.2955100e+01 8.3812900e+01 9.0356000e+01
9.8107400e+01 1.1120120e+02 1.1943340e+02 1.2760880e+02 1.3192120e+02
1.3655740e+02 1.4435640e+02 1.4439970e+02 1.4568880e+02 1.4884480e+02
1.5079620e+02 1.6462380e+02 1.6809440e+02 1.7317920e+02 1.8871590e+02
1.9013320e+02 1.9818800e+02 2.0428300e+02 2.1297010e+02 2.1369770e+02
2.1727810e+02 2.1982000e+02 2.2918310e+02 2.3100950e+02 2.3337140e+02
2.3523850e+02 2.4782830e+02 2.5512870e+02 2.6587170e+02 2.7834730e+02
2.8176940e+02 2.8611080e+02 2.9607380e+02 2.9909440e+02 3.1118600e+02
3.1505370e+02 3.1625390e+02 3.1800260e+02 3.2195310e+02 3.2526100e+02
3.3206010e+02 3.4202720e+02 3.6198760e+02 3.6305630e+02 3.6577470e+02
3.7129790e+02 3.7668200e+02 3.7791180e+02 3.7980260e+02 3.8990750e+02
3.9465220e+02 4.0668800e+02 4.0946490e+02 4.2851860e+02 4.3177020e+02
4.3948840e+02 4.5107180e+02 4.5600560e+02 4.6177160e+02 4.7193500e+02

4.7573790e+02 4.8067420e+02 4.8426500e+02 4.8509360e+02 4.8769580e+02
4.9164760e+02 4.9755310e+02 5.0761250e+02 5.2194580e+02 5.2759660e+02
5.2909660e+02 5.3396620e+02 5.4165150e+02 5.5424640e+02 5.6319520e+02
5.7208140e+02 5.7923610e+02 5.8679460e+02 5.9237480e+02 5.9530900e+02
5.9926920e+02 6.0222490e+02 6.0922210e+02 6.1539740e+02 6.1995820e+02
6.2122520e+02 6.2278810e+02 6.2789650e+02 6.2914220e+02 6.3023900e+02
6.3060500e+02 6.3588940e+02 6.4332080e+02 6.4693130e+02 6.4813460e+02
6.4975810e+02 6.5781420e+02 6.6585960e+02 6.7836140e+02 6.8418160e+02
6.9551300e+02 7.0446910e+02 7.0489370e+02 7.0561780e+02 7.2947140e+02
7.3926280e+02 7.3980760e+02 7.4281490e+02 7.4384470e+02 7.4404480e+02
7.4437110e+02 7.4508570e+02 7.4520660e+02 7.4560220e+02 7.4682660e+02
7.4772690e+02 7.5134640e+02 7.5880540e+02 7.5973650e+02 7.6032900e+02
7.8726110e+02 7.8758940e+02 7.8806950e+02 8.0013010e+02 8.0033470e+02
8.0055250e+02 8.1194050e+02 8.1264940e+02 8.1286340e+02 8.1476070e+02
8.1567890e+02 8.1605320e+02 8.2010820e+02 8.2218770e+02 8.2341360e+02
8.2554200e+02 8.2684000e+02 8.4100790e+02 8.4131530e+02 8.4833480e+02
8.4955870e+02 8.6488230e+02 8.6819400e+02 8.6833570e+02 8.8305250e+02
8.8876610e+02 8.9036390e+02 8.9071120e+02 8.9808430e+02 9.0510810e+02
9.0689760e+02 9.1712460e+02 9.1721510e+02 9.1939400e+02 9.2080370e+02
9.2178730e+02 9.2237660e+02 9.2307250e+02 9.2420890e+02 9.3370820e+02
9.5248600e+02 9.5256770e+02 9.5697070e+02 9.6707340e+02 9.6746570e+02
9.6787500e+02 1.0141364e+03 1.0141997e+03 1.0148882e+03 1.0226648e+03
1.0231361e+03 1.0235752e+03 1.0664950e+03 1.0694216e+03 1.0699743e+03
1.0706734e+03 1.0718060e+03 1.0737640e+03 1.0773052e+03 1.0824493e+03
1.0860031e+03 1.0870643e+03 1.0881602e+03 1.0980283e+03 1.0981390e+03
1.0983804e+03 1.1020376e+03 1.1028753e+03 1.1057004e+03 1.1175522e+03
1.1178780e+03 1.1178951e+03 1.2005720e+03 1.2007188e+03 1.2103532e+03
1.2112315e+03 1.2128140e+03 1.2134940e+03 1.2207368e+03 1.2235531e+03
1.2321570e+03 1.2343899e+03 1.2358387e+03 1.2386130e+03 1.2443248e+03
1.2454749e+03 1.2503172e+03 1.2549051e+03 1.2555367e+03 1.2565159e+03
1.2593267e+03 1.2612612e+03 1.2706555e+03 1.2747758e+03 1.2751648e+03
1.2919875e+03 1.2946610e+03 1.3190539e+03 1.3349264e+03 1.3366136e+03
1.3419588e+03 1.3541850e+03 1.3587292e+03 1.3657891e+03 1.3766476e+03
1.3771400e+03 1.3772990e+03 1.3794470e+03 1.3797464e+03 1.3799727e+03
1.3818898e+03 1.3914059e+03 1.4021913e+03 1.4025260e+03 1.4028226e+03
1.4029507e+03 1.4064344e+03 1.4142528e+03 1.4176603e+03 1.4253841e+03
1.4257017e+03 1.4263791e+03 1.4405093e+03 1.4424804e+03 1.4434625e+03

1.4582719e+03 1.4585909e+03 1.4591408e+03 1.4652885e+03 1.4661199e+03
1.4661542e+03 1.4662630e+03 1.4666902e+03 1.4679158e+03 1.4744489e+03
1.4779830e+03 1.4780141e+03 1.4781887e+03 1.4827049e+03 1.4839966e+03
1.4853922e+03 1.4935983e+03 1.4954530e+03 1.5002981e+03 1.5019759e+03
1.5023527e+03 1.5330300e+03 1.5360259e+03 1.5476478e+03 1.5498654e+03
1.5614292e+03 1.5661424e+03 1.5873373e+03 1.5919277e+03 1.5974232e+03
1.6007410e+03 1.6043703e+03 1.6056167e+03 1.6444104e+03 1.6451935e+03
1.6462594e+03 1.8004663e+03 1.8013556e+03 1.8027574e+03 1.8460480e+03
1.8466463e+03 1.8482491e+03 3.0386490e+03 3.0387078e+03 3.0388000e+03
3.0729123e+03 3.0730011e+03 3.0735870e+03 3.1218643e+03 3.1219216e+03
3.1222283e+03 3.1252768e+03 3.1253460e+03 3.1253612e+03 3.1409342e+03
3.1409731e+03 3.1412887e+03 3.1644569e+03 3.1644715e+03 3.1654105e+03
3.2058853e+03 3.2059154e+03 3.2061526e+03 3.2071502e+03 3.2072522e+03
3.2081610e+03 3.2082752e+03 3.2082930e+03 3.2107100e+03 3.2188379e+03
3.2188717e+03 3.2189416e+03 3.2250559e+03 3.2257797e+03 3.2261418e+03
3.2403823e+03 3.2502745e+03 3.2506575e+03 3.2508531e+03 3.2509034e+03]

Calculations for **P2**:

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[Geometry 52]

O	-21.0529940000	-2.7796640000	0.1686410000
C	-20.0366820000	-2.1293080000	0.2873070000
N	-20.0145060000	-0.7749160000	0.6250680000
C	-21.2114730000	0.0208390000	0.8644270000
C	-21.7290800000	0.7225060000	-0.3906450000
C	-18.7204770000	-0.2689270000	0.7053440000
C	-17.7997020000	-1.4140760000	0.3721510000
C	-18.6139540000	-2.5441000000	0.1250130000
C	-18.0569360000	-3.7897690000	-0.2210970000
C	-18.7221580000	-5.0607750000	-0.5113850000
C	-18.0190690000	-6.2156330000	-0.8462330000
C	-18.8343820000	-7.3394860000	-1.0701130000
C	-20.1897970000	-7.0748650000	-0.9095530000
C	-21.2947100000	-8.0018980000	-1.1024810000
C	-22.5623550000	-8.0584080000	-0.5283080000
C	-23.1362550000	-7.0963010000	0.4846150000
C	-24.0289090000	-6.0045860000	-0.1280000000

C	-23.3100100000	-9.1823470000	-1.0060260000
C	-22.6348430000	-9.9559000000	-1.9133650000
S	-21.0590540000	-9.3316730000	-2.2270190000
S	-20.4426220000	-5.3994510000	-0.4926030000
N	-16.6992180000	-3.8525060000	-0.3081430000
C	-15.9478540000	-2.8049130000	-0.0836010000
C	-16.3978500000	-1.4908250000	0.2708800000
C	-15.4069900000	-0.4382560000	0.4692800000
C	-15.5290690000	0.8542610000	0.9612420000
C	-14.3092290000	1.5601510000	1.0261220000
C	-13.2079580000	0.8384040000	0.5820170000
S	-13.7185570000	-0.7496070000	0.0637110000
C	-11.8360660000	1.2980400000	0.4863180000
S	-11.5672900000	3.0327440000	0.3975550000
C	-10.6229760000	0.6082650000	0.4696590000
C	-10.4399200000	-0.8898480000	0.5182330000
C	-10.2659850000	-1.5369050000	-0.8657360000
C	-9.5097560000	1.4920020000	0.4079860000
C	-9.8333850000	2.8368330000	0.3752970000
C	-8.9537090000	3.9830890000	0.3227750000
C	-9.2587950000	5.3207470000	0.5131220000
C	-8.1535480000	6.2073520000	0.3975030000
C	-8.2505180000	7.7033320000	0.5990270000
C	-9.4776170000	8.1797630000	1.3804040000
C	-6.9687340000	5.5234280000	0.1125350000
S	-7.2559710000	3.7995500000	-0.0290900000
C	-5.6232860000	6.0345480000	-0.0616000000
S	-4.2382290000	5.0310540000	0.2993130000
C	-5.2138390000	7.2872050000	-0.5099490000
C	-3.8109440000	7.4348250000	-0.5727780000
C	-3.1203400000	6.2990390000	-0.1745180000
C	-1.7025700000	5.9848710000	-0.0779690000
N	-1.4486850000	4.7210960000	0.3585130000
C	-0.2252210000	4.2738430000	0.5108690000
C	-0.5938800000	6.8037510000	-0.3761190000
C	0.7190050000	6.3133940000	-0.2074800000
C	1.6686500000	7.4163830000	-0.5769260000

N	0.8766060000	8.5022560000	-0.9390230000
C	1.4110770000	9.7907860000	-1.3602350000
C	1.6040370000	10.7700570000	-0.2029760000
C	-0.4901750000	8.2192880000	-0.8545060000
O	-1.3531840000	9.0242310000	-1.1353640000
O	2.8799130000	7.4183920000	-0.5871850000
C	0.9731950000	5.0164050000	0.2639870000
C	2.2514110000	4.3552690000	0.5275020000
C	2.4359800000	3.2926630000	1.4080590000
C	3.7472870000	2.7782680000	1.4244880000
C	4.6055350000	3.4268410000	0.5427010000
S	3.7575610000	4.7044910000	-0.2906460000
C	6.0044450000	3.1265530000	0.3004550000
S	6.5635090000	1.5045860000	0.6811630000
C	7.0530830000	3.9127370000	-0.1781340000
C	6.9693670000	5.3547320000	-0.6196410000
C	6.7948570000	5.5279640000	-2.1373970000
C	8.2807170000	3.1938960000	-0.2141700000
C	8.2042940000	1.8826690000	0.2201890000
C	9.2544880000	0.8934960000	0.3160660000
C	9.1788330000	-0.4156480000	0.7571370000
C	10.4053710000	-1.1354290000	0.7192420000
C	10.4887380000	-2.5757420000	1.1661730000
C	10.6967770000	-2.7463810000	2.6800570000
C	11.4538220000	-0.3526230000	0.2326700000
S	10.8928020000	1.2676640000	-0.1547530000
C	12.8516610000	-0.6540320000	-0.0112120000
S	13.6998660000	-1.9301400000	0.8284350000
C	13.7140810000	0.0172480000	-0.8739160000
C	15.0219530000	-0.4956620000	-0.8632480000
C	15.2050400000	-1.5702600000	0.0046100000
C	16.4907220000	-2.2539360000	0.1512420000
N	17.4766090000	-1.7332790000	-0.6313210000
C	18.6894750000	-2.2234570000	-0.6230590000
C	16.8394130000	-3.3447450000	0.9691820000
C	18.1518200000	-3.8740060000	0.9767170000
C	18.1606980000	-5.0174470000	1.9577490000

N	16.8699360000	-5.0987610000	2.4726150000
C	16.4508800000	-6.0915550000	3.4534820000
C	15.9735910000	-7.3987110000	2.8217780000
C	16.0194210000	-4.1337640000	1.9317870000
O	14.8514200000	-4.0147150000	2.2355280000
O	19.0577320000	-5.7624080000	2.2942360000
C	19.1622760000	-3.3262120000	0.1628130000
C	20.5576160000	-3.7306330000	0.0352030000
C	21.2829210000	-4.7331400000	0.6659250000
C	22.6315940000	-4.8036900000	0.2630980000
C	22.9955400000	-3.8605270000	-0.6914880000
S	21.6113810000	-2.8686350000	-1.0860580000
C	24.3009430000	-3.6836030000	-1.2987990000
C	24.7586090000	-2.7684660000	-2.2501280000
C	23.9081040000	-1.6919440000	-2.8871420000
C	24.6248110000	-0.7980630000	-3.9007220000
C	26.1411730000	-2.9699970000	-2.5553070000
C	26.7178470000	-4.0024360000	-1.8616120000
S	25.5927070000	-4.7684960000	-0.8084380000
O	-18.4722260000	0.8811000000	1.0026550000
H	-20.9574880000	0.7573010000	1.6408120000
H	-21.9721720000	-0.6647090000	1.2651600000
H	-20.9748760000	1.4147950000	-0.7950900000
H	-21.9936300000	-0.0079280000	-1.1705810000
H	-22.6319510000	1.3055470000	-0.1496760000
H	-16.9325460000	-6.2133700000	-0.9070880000
H	-18.4495140000	-8.3284420000	-1.3232630000
H	-22.3246280000	-6.6243580000	1.0597620000
H	-23.7294170000	-7.6787800000	1.2104050000
H	-24.4520020000	-5.3611320000	0.6599140000
H	-24.8655650000	-6.4440630000	-0.6946340000
H	-23.4590130000	-5.3602050000	-0.8148620000
H	-24.3229970000	-9.4071310000	-0.6657950000
H	-22.9785860000	-10.8588470000	-2.4162750000
H	-14.8689400000	-2.9798390000	-0.1748400000
H	-16.4883000000	1.2658210000	1.2654180000
H	-14.2278570000	2.5783460000	1.4091710000

H	-9.5477110000	-1.1059100000	1.1298850000
H	-11.2881480000	-1.3581020000	1.0413190000
H	-10.1104140000	-2.6235810000	-0.7714390000
H	-9.3978200000	-1.1146890000	-1.3963040000
H	-11.1526390000	-1.3754980000	-1.4984410000
H	-8.4768490000	1.1375910000	0.4148650000
H	-10.2681470000	5.6523090000	0.7575390000
H	-8.2423080000	8.2020060000	-0.3881350000
H	-7.3349280000	8.0495250000	1.1065030000
H	-9.4347890000	9.2694780000	1.5315370000
H	-10.4171810000	7.9623130000	0.8482570000
H	-9.5348650000	7.7046250000	2.3727350000
H	-5.9054020000	8.0664700000	-0.8254390000
H	-3.3016210000	8.3357150000	-0.9081490000
H	-0.1393770000	3.2316490000	0.8358510000
H	0.7090870000	10.2020190000	-2.1001720000
H	2.3700330000	9.5890830000	-1.8595170000
H	2.0091430000	11.7222800000	-0.5802140000
H	0.6470290000	10.9820100000	0.2978960000
H	2.3111970000	10.3697210000	0.5396630000
H	1.6454710000	2.9157610000	2.0573590000
H	4.0726910000	1.9727970000	2.0840370000
H	6.1480260000	5.8678000000	-0.0957920000
H	7.8969290000	5.8623040000	-0.3049310000
H	6.7637170000	6.5960300000	-2.4051270000
H	5.8588020000	5.0663160000	-2.4879980000
H	7.6252750000	5.0609530000	-2.6907110000
H	9.2162810000	3.6482420000	-0.5472010000
H	8.2447310000	-0.8677170000	1.0974580000
H	9.5509200000	-3.0777370000	0.8735750000
H	11.2949990000	-3.0942770000	0.6246360000
H	10.7164570000	-3.8139820000	2.9507740000
H	11.6494110000	-2.3020260000	3.0065040000
H	9.8868160000	-2.2640150000	3.2503460000
H	13.3937350000	0.8446540000	-1.5087920000
H	15.8419110000	-0.1209300000	-1.4726530000
H	19.3957510000	-1.7204710000	-1.2945370000

H	17.3113280000	-6.2743770000	4.1136370000
H	15.6459290000	-5.6313110000	4.0445770000
H	16.7761080000	-7.8680550000	2.2324750000
H	15.6700390000	-8.1072290000	3.6085610000
H	15.1065640000	-7.2267480000	2.1655800000
H	20.8311880000	-5.3938250000	1.4019270000
H	23.3326420000	-5.5361010000	0.6659150000
H	23.4768550000	-1.0583080000	-2.0913470000
H	23.0388280000	-2.1656100000	-3.3779090000
H	23.9281370000	-0.0489340000	-4.3070340000
H	25.4660990000	-0.2539370000	-3.4427840000
H	25.0195130000	-1.3780420000	-4.7500540000
H	26.6940030000	-2.3635870000	-3.2719350000
H	27.7470040000	-4.3548020000	-1.9136810000

Vibrational Frequencies(cm^-1)

[1.5324000e+00 2.3222000e+00 3.2056000e+00 3.8564000e+00 5.0780000e+00
6.1328000e+00 6.5564000e+00 8.9157000e+00 9.1714000e+00 1.0633800e+01
1.1248300e+01 1.2351300e+01 1.4285300e+01 1.5248400e+01 1.8533000e+01
1.9768500e+01 2.2350200e+01 2.5811400e+01 2.7221900e+01 2.8286300e+01
2.9730900e+01 3.0927200e+01 3.6845300e+01 4.0416600e+01 4.1739300e+01
4.2983500e+01 4.3705500e+01 4.5599700e+01 5.0027500e+01 5.0708700e+01
5.2331000e+01 5.4389700e+01 5.7270000e+01 6.0284500e+01 6.3593300e+01
6.7638500e+01 7.0316100e+01 7.1259400e+01 7.3579700e+01 7.6119800e+01
7.9093600e+01 8.0127000e+01 8.1398400e+01 8.3431200e+01 8.4510900e+01
8.8285400e+01 9.1756600e+01 9.3007500e+01 9.3991900e+01 9.8763700e+01
1.1183580e+02 1.1485410e+02 1.1748720e+02 1.2036420e+02 1.2258320e+02
1.2358450e+02 1.2830130e+02 1.3058400e+02 1.3354650e+02 1.3648110e+02
1.4202300e+02 1.4335210e+02 1.4570950e+02 1.4704500e+02 1.4710790e+02
1.5077390e+02 1.5462330e+02 1.5810690e+02 1.7092040e+02 1.7524100e+02
1.8376260e+02 1.8840590e+02 1.9261130e+02 1.9388370e+02 1.9815450e+02
1.9939860e+02 2.0105770e+02 2.0277800e+02 2.0380040e+02 2.0820170e+02
2.1108050e+02 2.1323470e+02 2.1572310e+02 2.2037830e+02 2.2664240e+02
2.3025300e+02 2.3369760e+02 2.3542390e+02 2.3907560e+02 2.4208580e+02
2.4403380e+02 2.5377940e+02 2.5798200e+02 2.6335720e+02 2.6822200e+02
2.7152560e+02 2.7831440e+02 2.8105650e+02 2.8423860e+02 2.8869210e+02
2.8983810e+02 2.9006330e+02 2.9170840e+02 3.0217460e+02 3.0879430e+02

3.0965330e+02 3.1315110e+02 3.1747830e+02 3.2076760e+02 3.2325410e+02
3.2407760e+02 3.2458310e+02 3.2647180e+02 3.3930080e+02 3.4252730e+02
3.5186910e+02 3.5262930e+02 3.5424830e+02 3.5776480e+02 3.6572270e+02
3.7081030e+02 3.7299410e+02 3.7654690e+02 3.7701950e+02 3.8196890e+02
3.9066170e+02 3.9261030e+02 4.0140110e+02 4.0270070e+02 4.1562600e+02
4.2185300e+02 4.2540810e+02 4.3164380e+02 4.3220830e+02 4.3872690e+02
4.4622790e+02 4.4852090e+02 4.4931420e+02 4.5861120e+02 4.6922520e+02
4.7351930e+02 4.7942390e+02 4.8067020e+02 4.8633070e+02 4.8809850e+02
4.8976640e+02 4.9191490e+02 4.9965440e+02 5.0221360e+02 5.0480710e+02
5.0672140e+02 5.2336490e+02 5.2651160e+02 5.2673820e+02 5.3275160e+02
5.3487730e+02 5.3965120e+02 5.5422960e+02 5.5446350e+02 5.5807210e+02
5.6273310e+02 5.6487980e+02 5.6786490e+02 5.7428300e+02 5.8976820e+02
5.9572060e+02 5.9906490e+02 6.0016050e+02 6.0266170e+02 6.0725850e+02
6.1006450e+02 6.1261440e+02 6.1573110e+02 6.1787030e+02 6.2007680e+02
6.2133290e+02 6.2535090e+02 6.3239320e+02 6.3324580e+02 6.3581060e+02
6.4667340e+02 6.5001220e+02 6.5013670e+02 6.5244050e+02 6.5533460e+02
6.6255180e+02 6.6419360e+02 6.6640930e+02 6.6821780e+02 6.7576090e+02
6.7936430e+02 6.8416510e+02 6.8981940e+02 6.9249160e+02 7.0055440e+02
7.0068210e+02 7.0126210e+02 7.0294550e+02 7.0626410e+02 7.1497900e+02
7.2893020e+02 7.2983950e+02 7.3028960e+02 7.4146720e+02 7.4228700e+02
7.4383450e+02 7.4400670e+02 7.4451150e+02 7.4564340e+02 7.4742370e+02
7.4810440e+02 7.4903290e+02 7.5833760e+02 7.5845370e+02 7.5959300e+02
7.8847690e+02 7.8872270e+02 7.8873500e+02 7.9029510e+02 7.9055590e+02
7.9150280e+02 7.9243300e+02 7.9471140e+02 7.9526830e+02 7.9627400e+02
7.9717690e+02 8.0779190e+02 8.1089440e+02 8.1103200e+02 8.1349130e+02
8.1639400e+02 8.1761420e+02 8.1941380e+02 8.2715610e+02 8.4017610e+02
8.4060490e+02 8.4237390e+02 8.4296940e+02 8.4329930e+02 8.4488230e+02
8.4619110e+02 8.4801850e+02 8.4884830e+02 8.6315530e+02 8.6486280e+02
8.7329620e+02 8.7538780e+02 8.7918750e+02 8.7928550e+02 8.7946520e+02
8.8137250e+02 8.8161410e+02 8.9146310e+02 8.9203730e+02 8.9212680e+02
9.1063830e+02 9.1170800e+02 9.1172690e+02 9.1329270e+02 9.1490400e+02
9.1766870e+02 9.2138150e+02 9.2540820e+02 9.2628370e+02 9.3094050e+02
9.3575240e+02 9.4379430e+02 9.4532000e+02 9.4848120e+02 9.4992950e+02
9.5662350e+02 9.5715940e+02 9.6622220e+02 9.6846280e+02 9.7150230e+02
9.7594080e+02 1.0046969e+03 1.0112314e+03 1.0122530e+03 1.0168958e+03
1.0177461e+03 1.0179996e+03 1.0185565e+03 1.0188146e+03 1.0237031e+03
1.0244625e+03 1.0249469e+03 1.0264306e+03 1.0693092e+03 1.0693926e+03

1.0697921e+03 1.0704676e+03 1.0710663e+03 1.0714838e+03 1.0717133e+03
1.0789448e+03 1.0801154e+03 1.0822933e+03 1.0835075e+03 1.0845028e+03
1.0845932e+03 1.0852618e+03 1.0870568e+03 1.0889406e+03 1.0913842e+03
1.0922348e+03 1.0983033e+03 1.0989015e+03 1.0990645e+03 1.0997497e+03
1.1038473e+03 1.1047723e+03 1.1062495e+03 1.1095791e+03 1.1213795e+03
1.1217371e+03 1.1238603e+03 1.1906099e+03 1.1966821e+03 1.1980180e+03
1.1994421e+03 1.2071221e+03 1.2085306e+03 1.2121982e+03 1.2136043e+03
1.2141730e+03 1.2191351e+03 1.2197577e+03 1.2257643e+03 1.2286516e+03
1.2313285e+03 1.2328993e+03 1.2357719e+03 1.2385696e+03 1.2404885e+03
1.2438381e+03 1.2483854e+03 1.2501811e+03 1.2540614e+03 1.2547755e+03
1.2587476e+03 1.2620259e+03 1.2679176e+03 1.2708165e+03 1.2714231e+03
1.2759001e+03 1.2815220e+03 1.2822913e+03 1.2831575e+03 1.2868092e+03
1.2896200e+03 1.2913819e+03 1.3097287e+03 1.3139256e+03 1.3167923e+03
1.3275297e+03 1.3325127e+03 1.3364258e+03 1.3437116e+03 1.3480424e+03
1.3494249e+03 1.3503647e+03 1.3550045e+03 1.3564754e+03 1.3676930e+03
1.3715725e+03 1.3740236e+03 1.3769808e+03 1.3770202e+03 1.3785870e+03
1.3786378e+03 1.3800202e+03 1.3804709e+03 1.3806216e+03 1.3890263e+03
1.3922360e+03 1.3949281e+03 1.3960307e+03 1.3966819e+03 1.3976406e+03
1.3982142e+03 1.3988302e+03 1.4015673e+03 1.4027187e+03 1.4028639e+03
1.4029346e+03 1.4032289e+03 1.4156829e+03 1.4171999e+03 1.4210536e+03
1.4256448e+03 1.4266811e+03 1.4340231e+03 1.4360588e+03 1.4372221e+03
1.4389478e+03 1.4403973e+03 1.4523728e+03 1.4569212e+03 1.4572853e+03
1.4585629e+03 1.4593935e+03 1.4631495e+03 1.4640492e+03 1.4649506e+03
1.4650766e+03 1.4660060e+03 1.4660096e+03 1.4660120e+03 1.4665389e+03
1.4671874e+03 1.4674697e+03 1.4681804e+03 1.4684532e+03 1.4709497e+03
1.4714035e+03 1.4741433e+03 1.4750105e+03 1.4755286e+03 1.4768199e+03
1.4779244e+03 1.4779586e+03 1.4784140e+03 1.4789025e+03 1.4801583e+03
1.4829082e+03 1.4833632e+03 1.4836691e+03 1.4841222e+03 1.4842765e+03
1.4863939e+03 1.4887282e+03 1.4902856e+03 1.4928188e+03 1.4938023e+03
1.4964747e+03 1.4969370e+03 1.4979830e+03 1.4991481e+03 1.5400436e+03
1.5428737e+03 1.5507101e+03 1.5572841e+03 1.5586788e+03 1.5724537e+03
1.5787901e+03 1.5812059e+03 1.5841338e+03 1.5869948e+03 1.5887296e+03
1.5913450e+03 1.5974863e+03 1.6087429e+03 1.6108703e+03 1.6408001e+03
1.6414210e+03 1.6442514e+03 1.7939674e+03 1.7947848e+03 1.7978087e+03
1.8384818e+03 1.8394990e+03 1.8432580e+03 3.0118899e+03 3.0141067e+03
3.0311785e+03 3.0313773e+03 3.0318665e+03 3.0325204e+03 3.0338642e+03
3.0338935e+03 3.0358392e+03 3.0386917e+03 3.0387001e+03 3.0387066e+03

3.0391050e+03 3.0397906e+03 3.0407418e+03 3.0479344e+03 3.0660644e+03
3.0736292e+03 3.0737090e+03 3.0740761e+03 3.0888856e+03 3.0890634e+03
3.0898597e+03 3.0900040e+03 3.1133900e+03 3.1148146e+03 3.1149947e+03
3.1151192e+03 3.1155134e+03 3.1161655e+03 3.1170972e+03 3.1176595e+03
3.1204253e+03 3.1211172e+03 3.1222198e+03 3.1224439e+03 3.1224785e+03
3.1232499e+03 3.1244037e+03 3.1251452e+03 3.1251867e+03 3.1252834e+03
3.1413501e+03 3.1415338e+03 3.1416759e+03 3.1428102e+03 3.1435781e+03
3.1661763e+03 3.1964928e+03 3.1972554e+03 3.1979592e+03 3.1997080e+03
3.2094925e+03 3.2096145e+03 3.2104114e+03 3.2108078e+03 3.2124867e+03
3.2173750e+03 3.2237376e+03 3.2257065e+03 3.2350883e+03 3.2471673e+03
3.2500134e+03 3.2505487e+03 3.2508041e+03 3.2517474e+03 3.2533589e+03
3.2557496e+03]

Calculations for **P3**:

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[Geometry 106]

C	-22.5718250000	-7.6563860000	2.7944250000
C	-23.1102530000	-6.4213390000	3.5158170000
N	-23.4423130000	-5.3270140000	2.6126680000
C	-22.5420670000	-4.3368380000	2.2318040000
O	-21.3957130000	-4.2673480000	2.6170130000
C	-23.2851170000	-3.4392430000	1.2850770000
C	-22.8731180000	-2.2658970000	0.6349800000
C	-23.8964320000	-1.7099360000	-0.1974540000
N	-25.1117540000	-2.1821060000	-0.3381080000
C	-25.5285100000	-3.3008420000	0.3159190000
C	-26.9122900000	-3.6582320000	0.0467590000
C	-27.7245940000	-4.6928630000	0.4897590000
C	-29.0297290000	-4.6429130000	-0.0455010000
C	-29.2381770000	-3.5714710000	-0.9052260000
S	-27.7937740000	-2.6062850000	-1.0513180000
C	-30.4459470000	-3.2211230000	-1.6262700000
C	-30.6447460000	-2.2125860000	-2.5516370000
C	-31.9754020000	-2.1444670000	-3.0690790000
C	-32.4286440000	-1.1465780000	-4.1069260000
C	-31.8540740000	-1.4079960000	-5.5070800000
C	-32.7761480000	-3.1203960000	-2.5188930000

S	-31.9339000000	-4.1124980000	-1.3809130000
C	-24.5907180000	-3.9561360000	1.1409850000
C	-24.6900100000	-5.1800870000	1.9980200000
O	-25.6156080000	-5.9413010000	2.1858660000
C	-21.5890600000	-1.5660510000	0.6974560000
C	-21.4016120000	-0.2203180000	0.3916980000
C	-20.0571870000	0.2014230000	0.4366770000
C	-19.1786140000	-0.8203620000	0.7692150000
S	-20.0420820000	-2.3079090000	1.0534470000
C	-17.7399960000	-0.7624130000	0.9179480000
C	-16.8867750000	-1.6816170000	1.5006660000
C	-15.5124740000	-1.3098850000	1.4968730000
C	-14.4496840000	-2.1912750000	2.1084100000
C	-13.9761900000	-3.3240960000	1.1832250000
C	-15.3100180000	-0.0699950000	0.8924100000
S	-16.8275680000	0.5988480000	0.3156940000
C	-14.1081170000	0.7215490000	0.6955550000
C	-14.0140350000	2.1014990000	0.5884940000
C	-12.7054800000	2.5694360000	0.3288780000
C	-11.7564810000	1.5624150000	0.2276090000
S	-12.5253070000	0.0047260000	0.4641050000
C	-10.3255260000	1.7138330000	0.0306360000
C	-9.3792630000	0.8764220000	-0.5597330000
C	-9.6357110000	-0.4914520000	-1.1459400000
C	-9.2880930000	-1.6483850000	-0.1950470000
C	-8.0836280000	1.4644360000	-0.5707540000
C	-8.0097000000	2.7260910000	-0.0076970000
S	-9.5823890000	3.2056070000	0.5815100000
C	-6.8625590000	3.5967170000	0.1266070000
C	-6.8294180000	4.9132730000	0.5726910000
C	-5.5353970000	5.4753360000	0.5782210000
C	-4.5557400000	4.5967790000	0.1353700000
S	-5.2607550000	3.0436150000	-0.2873680000
C	-3.1166820000	4.7223750000	-0.0344500000
C	-2.2882960000	5.8315120000	0.2348590000
C	-2.5865940000	7.2060480000	0.7492170000
O	-3.6353800000	7.7135120000	1.0870140000

N	-1.3639460000	7.8839550000	0.7793560000
C	-1.2115220000	9.2554730000	1.2477530000
C	-0.9690740000	9.3549830000	2.7533790000
C	-0.3044680000	7.0890530000	0.3525450000
O	0.8505150000	7.4514670000	0.3095600000
C	-0.9001820000	5.7598350000	-0.0111020000
C	-0.2957290000	4.6071630000	-0.5360120000
C	-1.2284350000	3.5396500000	-0.7365650000
N	-2.5190310000	3.5961540000	-0.5111850000
C	1.1032020000	4.3667380000	-0.8923430000
C	1.5391560000	3.3926830000	-1.7872750000
C	2.9410890000	3.2931490000	-1.8965010000
C	3.6143360000	4.1863380000	-1.0747470000
S	2.4878150000	5.1732400000	-0.1828600000
C	5.0419000000	4.3779770000	-0.9270800000
C	5.7225390000	5.4222620000	-0.3285730000
C	7.1424000000	5.3077780000	-0.3586930000
C	8.0383660000	6.4040890000	0.1698000000
C	7.9933360000	7.6847650000	-0.6785580000
C	7.5549550000	4.1416900000	-0.9982150000
S	6.1759610000	3.1942690000	-1.5276570000
C	8.8784690000	3.6077320000	-1.2868510000
C	9.2844990000	2.9232830000	-2.4210490000
C	10.6307770000	2.4891620000	-2.3769580000
C	11.2919190000	2.8253500000	-1.2047380000
S	10.1937410000	3.6712590000	-0.1316920000
C	12.6605830000	2.5044240000	-0.8390380000
C	13.5731600000	3.1473690000	-0.0028400000
C	13.3258410000	4.4044050000	0.7968770000
C	12.9537410000	4.1415510000	2.2652330000
C	14.8308910000	2.4821120000	0.0217200000
C	14.9080080000	1.3497300000	-0.7694240000
S	13.3749430000	1.0715880000	-1.5586160000
C	16.0285610000	0.4598400000	-0.9803880000
C	16.1467530000	-0.5779880000	-1.8973320000
C	17.3877090000	-1.2353370000	-1.8263290000
C	18.2480930000	-0.7215900000	-0.8584610000

S	17.4758200000	0.6113390000	-0.0178430000
C	19.5861350000	-1.2642270000	-0.6243090000
C	20.5664600000	-0.8562070000	0.2994660000
C	20.5645980000	0.2288260000	1.3240540000
O	19.7052730000	1.0406670000	1.5921660000
N	21.8008950000	0.1593610000	1.9728780000
C	22.2003290000	1.0492670000	3.0550470000
C	21.8290780000	0.5184540000	4.4392370000
C	22.6079140000	-0.8551390000	1.4641480000
O	23.7309390000	-1.0951520000	1.8499780000
C	21.8083630000	-1.5226400000	0.3829690000
C	22.1140910000	-2.6192830000	-0.4350220000
C	21.0569060000	-2.9256470000	-1.3541080000
N	19.9028540000	-2.3109830000	-1.4371830000
C	23.3144990000	-3.4539400000	-0.4692500000
C	23.3774140000	-4.7372100000	-1.0079940000
C	24.6664840000	-5.3064790000	-0.9992580000
C	25.6288740000	-4.4635180000	-0.4601410000
S	24.9114110000	-2.9633160000	0.0633420000
C	27.0439800000	-4.7070100000	-0.2814130000
C	27.9660120000	-3.9891830000	0.4585230000
C	29.2931140000	-4.5019720000	0.4247260000
C	30.4058590000	-3.8691330000	1.2305020000
C	30.6851360000	-4.5780200000	2.5651350000
C	29.3875730000	-5.6520480000	-0.3580100000
S	27.8332140000	-6.0500820000	-1.0680740000
C	30.5068780000	-6.5320760000	-0.6603460000
C	30.4447610000	-7.8500280000	-1.0862820000
C	31.7174900000	-8.4303270000	-1.3442760000
C	32.7529090000	-7.5602540000	-1.1132120000
S	32.1827810000	-6.0163340000	-0.5854750000
H	-23.3150810000	-8.0551780000	2.0872000000
H	-22.3391890000	-8.4467370000	3.5254380000
H	-21.6487360000	-7.4205570000	2.2429240000
H	-22.3653250000	-6.0327900000	4.2253910000
H	-24.0276590000	-6.6679370000	4.0698360000
H	-23.6622190000	-0.8243010000	-0.7971020000

H	-27.3687370000	-5.4562050000	1.1781690000
H	-29.8018760000	-5.3783400000	0.1868550000
H	-29.8478980000	-1.5302590000	-2.8551300000
H	-33.5298210000	-1.1508870000	-4.1539790000
H	-32.1403060000	-0.1319570000	-3.7797810000
H	-30.7525080000	-1.3825460000	-5.5013310000
H	-32.1600410000	-2.3973920000	-5.8825040000
H	-32.2032920000	-0.6477240000	-6.2241780000
H	-33.8303260000	-3.3066500000	-2.7224650000
H	-22.2250900000	0.4575540000	0.1670740000
H	-19.7376420000	1.2287800000	0.2559930000
H	-17.2456340000	-2.6054110000	1.9595570000
H	-14.8594210000	-2.6316930000	3.0332890000
H	-13.5864620000	-1.5817060000	2.4175370000
H	-13.5246670000	-2.9260070000	0.2610330000
H	-13.2221710000	-3.9501800000	1.6867290000
H	-14.8146000000	-3.9749480000	0.8879980000
H	-14.8778140000	2.7578860000	0.7035850000
H	-12.4545730000	3.6244520000	0.2098320000
H	-10.6873160000	-0.5756190000	-1.4612290000
H	-9.0330930000	-0.5896090000	-2.0648970000
H	-9.8958690000	-1.6094250000	0.7224550000
H	-9.4691990000	-2.6208930000	-0.6803400000
H	-8.2292260000	-1.6120970000	0.1068760000
H	-7.2168810000	0.9691840000	-1.0135670000
H	-7.7225690000	5.4599900000	0.8800370000
H	-5.3049310000	6.4915670000	0.8904000000
H	-0.3683230000	9.6894310000	0.6909180000
H	-2.1298740000	9.7923320000	0.9688470000
H	-0.0471180000	8.8265480000	3.0407910000
H	-1.8125170000	8.9284850000	3.3175820000
H	-0.8620390000	10.4109850000	3.0475530000
H	-0.8529300000	2.5731170000	-1.0879700000
H	0.8569560000	2.7800900000	-2.3766900000
H	3.4491410000	2.6055130000	-2.5741900000
H	5.2080520000	6.2799520000	0.1100640000
H	7.7337900000	6.6415400000	1.2042720000

H	9.0765880000	6.0502130000	0.2325410000
H	8.3339590000	7.4890960000	-1.7075570000
H	6.9731600000	8.0961390000	-0.7386620000
H	8.6439070000	8.4619520000	-0.2464140000
H	8.6260950000	2.7693570000	-3.2772270000
H	11.1237940000	1.9668590000	-3.1981180000
H	14.2423080000	5.0176670000	0.7636180000
H	12.5381710000	5.0067670000	0.3183700000
H	13.7430410000	3.5712460000	2.7803110000
H	12.8115490000	5.0898420000	2.8080740000
H	12.0202940000	3.5627160000	2.3451570000
H	15.6801850000	2.8514620000	0.6004570000
H	15.3593560000	-0.8428800000	-2.6048800000
H	17.6875800000	-2.0701790000	-2.4566430000
H	23.2888680000	1.1837440000	2.9724570000
H	21.7117000000	2.0168540000	2.8691300000
H	20.7400500000	0.3877790000	4.5325080000
H	22.3195180000	-0.4471590000	4.6364030000
H	22.1544170000	1.2301720000	5.2143570000
H	21.2131560000	-3.7307900000	-2.0795910000
H	22.5015230000	-5.2701600000	-1.3775340000
H	24.8863500000	-6.3140450000	-1.3551970000
H	27.6929700000	-3.1050700000	1.0385090000
H	31.3324700000	-3.8210240000	0.6374930000
H	30.1283780000	-2.8207570000	1.4278690000
H	31.4793820000	-4.0581630000	3.1246130000
H	29.7830140000	-4.6007780000	3.1966930000
H	31.0100280000	-5.6175920000	2.4051920000
H	29.5018300000	-8.3884210000	-1.1932190000
H	31.8594480000	-9.4593490000	-1.6778600000
H	33.8226330000	-7.7383080000	-1.2139590000

Vibrational Frequencies(cm^-1)

[1.0827000e+00 1.3599000e+00 1.9515000e+00 3.0611000e+00 3.8718000e+00
5.1078000e+00 5.5442000e+00 6.0458000e+00 7.3417000e+00 9.0565000e+00
1.0137200e+01 1.0791800e+01 1.2117400e+01 1.2278700e+01 1.4124600e+01
1.5093500e+01 1.6801800e+01 1.8354000e+01 1.9144000e+01 2.2911400e+01

2.4342700e+01 2.5275400e+01 2.6472900e+01 2.7890300e+01 2.9252900e+01
3.0838900e+01 3.4149600e+01 3.6577700e+01 4.0287200e+01 4.0797800e+01
4.2331700e+01 4.2838300e+01 4.3081100e+01 4.5116400e+01 4.6675100e+01
4.7486000e+01 4.8936000e+01 5.0343000e+01 5.1946600e+01 5.4539500e+01
5.5345900e+01 5.9504400e+01 6.1242500e+01 6.2111600e+01 6.5884700e+01
6.7560500e+01 6.9490900e+01 7.3955500e+01 7.5871000e+01 7.6713500e+01
8.1482200e+01 8.1947200e+01 8.5219200e+01 8.6589200e+01 9.0310300e+01
9.1114600e+01 9.4453500e+01 9.8061800e+01 1.0240430e+02 1.0844520e+02
1.0947890e+02 1.1631940e+02 1.1712560e+02 1.2270590e+02 1.2382320e+02
1.2715140e+02 1.2952580e+02 1.3160430e+02 1.3271270e+02 1.3596970e+02
1.3960190e+02 1.4498720e+02 1.4597880e+02 1.4636710e+02 1.4870400e+02
1.5179650e+02 1.5814320e+02 1.6980210e+02 1.7159720e+02 1.7309440e+02
1.7696630e+02 1.8201880e+02 1.8413600e+02 1.9300820e+02 1.9512850e+02
1.9918940e+02 2.0191130e+02 2.0615390e+02 2.0721110e+02 2.0926670e+02
2.1131240e+02 2.1221320e+02 2.1428250e+02 2.1683950e+02 2.2093490e+02
2.2298570e+02 2.2526480e+02 2.2880040e+02 2.3169900e+02 2.3547340e+02
2.3792760e+02 2.4137350e+02 2.4460840e+02 2.4526430e+02 2.6000890e+02
2.6186120e+02 2.6248050e+02 2.6588140e+02 2.7284760e+02 2.7756830e+02
2.7950370e+02 2.8575270e+02 2.8839260e+02 2.9284980e+02 2.9795630e+02
3.0116910e+02 3.0672320e+02 3.0885540e+02 3.1356220e+02 3.1529900e+02
3.1742650e+02 3.1884180e+02 3.1942010e+02 3.2014500e+02 3.2066000e+02
3.2204950e+02 3.2532220e+02 3.3977370e+02 3.4175070e+02 3.4338410e+02
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4.6275600e+02 4.7186780e+02 4.7767210e+02 4.7987050e+02 4.8147200e+02
4.8470840e+02 4.8873260e+02 4.9178970e+02 4.9614450e+02 4.9840180e+02
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5.2252090e+02 5.2675970e+02 5.3200750e+02 5.3295460e+02 5.3327570e+02
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5.5691500e+02 5.5913030e+02 5.6590180e+02 5.7081550e+02 5.8273570e+02
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7.8600150e+02 7.8751490e+02 7.8775200e+02 7.8807450e+02 7.8820520e+02
7.8919750e+02 7.9043200e+02 7.9047660e+02 7.9197510e+02 7.9198920e+02
7.9214070e+02 8.0046230e+02 8.1225660e+02 8.1227070e+02 8.1233060e+02
8.1532770e+02 8.1872380e+02 8.1877750e+02 8.2301120e+02 8.2427600e+02
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8.9051160e+02 8.9160370e+02 8.9191690e+02 8.9525240e+02 9.1396740e+02
9.1492340e+02 9.1823420e+02 9.1833620e+02 9.1972960e+02 9.1995170e+02
9.2003370e+02 9.2059160e+02 9.3157420e+02 9.3310790e+02 9.3422640e+02
9.3817150e+02 9.3935160e+02 9.4138550e+02 9.4206700e+02 9.5234860e+02
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1.1942802e+03 1.1944011e+03 1.1949366e+03 1.1952055e+03 1.2006474e+03
1.2088842e+03 1.2147079e+03 1.2155486e+03 1.2188046e+03 1.2199742e+03
1.2215612e+03 1.2250324e+03 1.2266427e+03 1.2278746e+03 1.2316820e+03
1.2333005e+03 1.2343773e+03 1.2361949e+03 1.2382910e+03 1.2434991e+03
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1.4654011e+03 1.4660955e+03 1.4662089e+03 1.4662149e+03 1.4662399e+03
1.4665244e+03 1.4667406e+03 1.4670838e+03 1.4673446e+03 1.4682031e+03
1.4682423e+03 1.4682824e+03 1.4687973e+03 1.4694579e+03 1.4779428e+03
1.4780712e+03 1.4781146e+03 1.4781249e+03 1.4784141e+03 1.4784732e+03
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1.4878128e+03 1.4882896e+03 1.4904047e+03 1.4908202e+03 1.4916118e+03
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1.5020035e+03 1.5030470e+03 1.5109033e+03 1.5418325e+03 1.5457046e+03
1.5483610e+03 1.5556835e+03 1.5624775e+03 1.5696201e+03 1.5728990e+03
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1.6051285e+03 1.6055548e+03 1.6089781e+03 1.6099990e+03 1.6123235e+03
1.6144895e+03 1.6443343e+03 1.6447760e+03 1.6448511e+03 1.7979810e+03
1.7981857e+03 1.8005149e+03 1.8436499e+03 1.8436965e+03 1.8455263e+03
3.0293938e+03 3.0296758e+03 3.0303579e+03 3.0306632e+03 3.0306916e+03
3.0309421e+03 3.0325165e+03 3.0355933e+03 3.0385208e+03 3.0387611e+03
3.0387824e+03 3.0393558e+03 3.0396829e+03 3.0399995e+03 3.0485726e+03
3.0725804e+03 3.0742322e+03 3.0742583e+03 3.0770770e+03 3.0888967e+03
3.0890024e+03 3.0892012e+03 3.0894196e+03 3.1048407e+03 3.1123095e+03
3.1141411e+03 3.1141887e+03 3.1143029e+03 3.1147141e+03 3.1149724e+03
3.1165644e+03 3.1188589e+03 3.1192045e+03 3.1195790e+03 3.1216574e+03
3.1225056e+03 3.1225178e+03 3.1239315e+03 3.1241264e+03 3.1249943e+03
3.1252900e+03 3.1253586e+03 3.1407177e+03 3.1416871e+03 3.1416935e+03
3.1646144e+03 3.1672855e+03 3.1679456e+03 3.1976819e+03 3.1978996e+03
3.1980483e+03 3.1982453e+03 3.1985008e+03 3.1987841e+03 3.2059352e+03

3.2062039e+03 3.2063647e+03 3.2064292e+03 3.2065094e+03 3.2075186e+03
3.2082104e+03 3.2082174e+03 3.2082926e+03 3.2186612e+03 3.2194241e+03
3.2197043e+03 3.2244000e+03 3.2246030e+03 3.2254787e+03 3.2383975e+03
3.2500615e+03 3.2505875e+03 3.2517959e+03 3.2523157e+03]

Calculations for **P4**:

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[Geometry 101]

C	28.4394990000	4.2536690000	0.9795370000
C	28.3129590000	3.2991170000	2.1662270000
N	27.9731730000	1.9373450000	1.7741180000
C	28.9167820000	0.9705970000	1.4399450000
O	30.1130710000	1.1730000000	1.4635160000
C	28.1401210000	-0.2715300000	1.0858650000
C	28.5538260000	-1.5504490000	0.6660360000
C	27.4472770000	-2.4340780000	0.4400000000
N	26.1785860000	-2.1484330000	0.5825720000
C	25.7651410000	-0.9139520000	0.9828560000
C	24.3106800000	-0.7872860000	1.0812770000
C	23.4471370000	-1.8419740000	0.7909130000
C	22.0855470000	-1.5285890000	0.9460800000
C	21.8736690000	-0.2191810000	1.3614720000
S	23.3865080000	0.6287130000	1.5521710000
C	20.6181090000	0.4480600000	1.6251800000
C	20.3933430000	1.6933430000	2.1851160000
C	19.0235980000	2.0526140000	2.3208440000
C	18.6073950000	3.3740010000	2.9221190000
C	18.6218270000	4.5417300000	1.9220430000
C	18.1732350000	1.0510190000	1.8506970000
S	19.0945780000	-0.3069690000	1.2260570000
C	16.7261370000	0.9512420000	1.8177680000
C	15.9594290000	-0.2059230000	1.8050410000
C	14.5669600000	0.0278320000	1.7299970000
C	14.2299320000	1.3714840000	1.6827880000
S	15.6776670000	2.3542710000	1.7096290000
C	12.9213240000	1.9844030000	1.6243150000
C	12.5684720000	3.3142500000	1.7934120000

C	11.1782890000	3.5503700000	1.6888820000
C	10.4293580000	2.4091430000	1.4377520000
S	11.4952580000	1.0209730000	1.3077150000
C	8.9944810000	2.3210270000	1.2409350000
C	8.0916350000	1.2778450000	1.4503370000
C	8.4243020000	-0.1120070000	1.9387120000
C	8.5690440000	-1.1473880000	0.8113580000
C	6.7549440000	1.6663980000	1.1568070000
C	6.6070390000	2.9739190000	0.7293240000
S	8.1669620000	3.7558550000	0.6583010000
C	5.4010790000	3.6839320000	0.3686210000
C	5.2350560000	5.0317260000	0.0849120000
C	3.9068040000	5.3907020000	-0.2307150000
C	3.0120710000	4.3289100000	-0.1979960000
S	3.8763180000	2.8490280000	0.2318870000
C	1.5766580000	4.2733350000	-0.4505290000
C	0.7015860000	5.3119580000	-0.8233780000
C	0.9327620000	6.7794490000	-1.0781640000
O	1.9491100000	7.4400290000	-1.0190720000
N	-0.3042960000	7.3137870000	-1.4249860000
C	-0.5202670000	8.7210970000	-1.7357900000
C	-0.8210830000	9.5713330000	-0.5020790000
C	-1.3188700000	6.3553380000	-1.4187210000
O	-2.4763520000	6.5941370000	-1.6889100000
C	-0.6759160000	5.0671470000	-1.0327890000
C	-1.2269220000	3.7811510000	-0.8766300000
N	-0.3709670000	2.7867430000	-0.5107400000
C	0.9026400000	3.0145270000	-0.3178690000
C	-2.6083940000	3.3308230000	-1.0474140000
C	-2.9919950000	2.0050740000	-0.8526720000
C	-4.3605830000	1.7659210000	-1.0665890000
C	-5.0609350000	2.9095150000	-1.4325300000
S	-4.0030030000	4.2950780000	-1.5019030000
C	-6.4690330000	3.0434440000	-1.7330810000
C	-7.1498590000	4.1296810000	-2.2539580000
C	-8.5451260000	3.9287690000	-2.4451480000
C	-9.4304550000	5.0118820000	-3.0143030000

C	-9.9101830000	6.0327030000	-1.9694580000
C	-8.9449400000	2.6487370000	-2.0590520000
S	-7.5821780000	1.7292990000	-1.4421300000
C	-10.2352390000	1.9866370000	-2.1036700000
C	-10.4825860000	0.6226980000	-2.1760720000
C	-11.8558230000	0.2857210000	-2.1619700000
C	-12.6974810000	1.3837650000	-2.0779290000
S	-11.7556010000	2.8561800000	-1.9923210000
C	-14.1429740000	1.4288460000	-2.0602150000
C	-14.9871790000	2.5196010000	-2.1972290000
C	-16.3602220000	2.1841220000	-2.1514840000
C	-16.6045230000	0.8289110000	-1.9788180000
S	-15.0814360000	-0.0329660000	-1.8480630000
C	-17.8927830000	0.1726910000	-1.8532110000
C	-18.3049330000	-1.1265690000	-2.1499920000
C	-17.4389870000	-2.2414920000	-2.6865330000
C	-16.9302040000	-3.2070140000	-1.6036050000
C	-19.6939250000	-1.3133350000	-1.9018610000
C	-20.3560960000	-0.1968290000	-1.4245580000
S	-19.2341580000	1.1290600000	-1.2448290000
C	-21.7543740000	-0.0410720000	-1.0865840000
C	-22.4658960000	1.1297060000	-0.8625270000
C	-23.8235490000	0.9005660000	-0.5621540000
C	-24.1898910000	-0.4436150000	-0.5574260000
S	-22.7954600000	-1.4324890000	-0.9462610000
C	-25.5152950000	-0.9476930000	-0.1984240000
C	-26.1229600000	-2.1716350000	-0.5106330000
C	-25.6110800000	-3.3470630000	-1.2919450000
O	-24.5250880000	-3.5178410000	-1.8012090000
N	-26.6499630000	-4.2733630000	-1.3238000000
C	-26.5683090000	-5.5627250000	-1.9971290000
C	-27.0166320000	-5.5091340000	-3.4571730000
C	-27.7796710000	-3.8269300000	-0.6311440000
O	-28.8001230000	-4.4709450000	-0.5168940000
C	-27.4424350000	-2.4709200000	-0.1073650000
C	-28.1985080000	-1.5481320000	0.6400190000
N	-27.5890510000	-0.3739580000	0.9670920000

C	-26.3644540000	-0.1022060000	0.5889410000
C	-29.5689070000	-1.6585320000	1.1382630000
C	-30.1829180000	-0.6505740000	1.8785150000
C	-31.5023680000	-0.9455270000	2.2649770000
C	-31.9306560000	-2.1931060000	1.8270810000
S	-30.6786730000	-3.0007580000	0.9197740000
C	-33.2136100000	-2.8284130000	2.0371350000
C	-33.5968280000	-4.1291430000	1.7644180000
C	-34.9422580000	-4.4428290000	2.1098740000
C	-35.5188780000	-5.8215660000	1.8920010000
C	-35.9921740000	-6.0749010000	0.4515530000
C	-35.6054190000	-3.3491960000	2.6619100000
S	-34.5565930000	-1.9449140000	2.7203070000
C	-36.9551310000	-3.2045380000	3.1879780000
C	-37.3799290000	-2.3602120000	4.2011030000
C	-38.7800650000	-2.4216980000	4.4462970000
C	-39.4250070000	-3.3097010000	3.6217030000
S	-38.3282590000	-4.0731280000	2.5266150000
C	26.7685860000	0.0395470000	1.2385460000
C	26.6652200000	1.4594350000	1.6803750000
O	25.6826090000	2.1247350000	1.9287610000
C	29.9060170000	-2.0504680000	0.4446930000
C	31.1457340000	-1.4607510000	0.6537720000
C	32.2389610000	-2.2898360000	0.3203480000
C	31.8718910000	-3.5391190000	-0.1573750000
S	30.1346290000	-3.6798950000	-0.1989210000
C	32.7160350000	-4.6311410000	-0.5889890000
C	32.3663840000	-5.9319460000	-0.9027100000
C	33.4537500000	-6.7708420000	-1.2793740000
C	33.2514550000	-8.2234380000	-1.6396930000
C	32.7837320000	-8.4440250000	-3.0873400000
C	34.6682310000	-6.0891330000	-1.2526150000
S	34.4376350000	-4.4145480000	-0.7857570000
C	36.0291790000	-6.5323940000	-1.5187600000
C	37.1986020000	-6.0525300000	-0.9514150000
C	38.3752850000	-6.6660850000	-1.4642370000
C	38.1063380000	-7.6115310000	-2.4225510000

S	36.4103200000	-7.7546110000	-2.7177290000
H	29.2329240000	3.9244740000	0.2912540000
H	28.6955070000	5.2639290000	1.3358810000
H	27.4921720000	4.3190140000	0.4226270000
H	27.5223070000	3.6372300000	2.8515920000
H	29.2608490000	3.2464390000	2.7214900000
H	27.6571190000	-3.4613830000	0.1183350000
H	23.8311930000	-2.8108710000	0.4782580000
H	21.2757920000	-2.2388560000	0.7710870000
H	21.2066950000	2.3399020000	2.5213050000
H	19.2963960000	3.6047360000	3.7522110000
H	17.6066510000	3.2857190000	3.3728350000
H	18.3376790000	5.4839230000	2.4176970000
H	17.9173320000	4.3692760000	1.0933430000
H	19.6230810000	4.6780180000	1.4833750000
H	16.4008190000	-1.2011170000	1.8742850000
H	13.8212940000	-0.7688360000	1.7364150000
H	13.2974300000	4.0957310000	2.0136600000
H	10.7224750000	4.5329320000	1.8191260000
H	9.3460880000	-0.0898780000	2.5404640000
H	7.6216850000	-0.4364020000	2.6226070000
H	7.6456290000	-1.2191820000	0.2148520000
H	9.3874990000	-0.8810340000	0.1244250000
H	8.7845580000	-2.1461340000	1.2237980000
H	5.9058920000	0.9916300000	1.2853540000
H	6.0576550000	5.7480280000	0.1142570000
H	3.5894400000	6.4010150000	-0.4774390000
H	-1.3576810000	8.7624290000	-2.4472590000
H	0.3878990000	9.0816850000	-2.2405130000
H	0.0153000000	9.5389690000	0.2127840000
H	-1.7340280000	9.2227300000	0.0047310000
H	-0.9755270000	10.6209600000	-0.7980080000
H	1.4902580000	2.1361270000	-0.0246130000
H	-2.2654790000	1.2480130000	-0.5644870000
H	-4.8275760000	0.7845330000	-0.9687120000
H	-6.6479220000	5.0615680000	-2.5227880000
H	-8.8629810000	5.5414020000	-3.7982770000

H	-10.3001730000	4.5629550000	-3.5187290000
H	-10.5278040000	6.8137310000	-2.4413730000
H	-10.5149400000	5.5505210000	-1.1855300000
H	-9.0586780000	6.5265890000	-1.4749320000
H	-9.6821130000	-0.1133650000	-2.2628310000
H	-12.2257070000	-0.7380570000	-2.2379510000
H	-14.6199050000	3.5351610000	-2.3534930000
H	-17.1632680000	2.9133540000	-2.2674760000
H	-16.5837830000	-1.8226640000	-3.2392740000
H	-18.0303980000	-2.8099530000	-3.4242250000
H	-17.7673040000	-3.6710950000	-1.0581710000
H	-16.3011860000	-2.6860180000	-0.8649060000
H	-16.3286080000	-4.0141990000	-2.0515390000
H	-20.2062250000	-2.2563510000	-2.1044000000
H	-22.0211170000	2.1230370000	-0.9380590000
H	-24.5305230000	1.7096920000	-0.3798180000
H	-25.5218610000	-5.8941460000	-1.9266810000
H	-27.1972160000	-6.2610640000	-1.4258820000
H	-26.3880670000	-4.8168120000	-4.0380480000
H	-26.9333720000	-6.5084820000	-3.9127760000
H	-28.0657860000	-5.1853760000	-3.5359980000
H	-25.9673760000	0.8568210000	0.9377580000
H	-29.6534420000	0.2686680000	2.1211100000
H	-32.1256190000	-0.2743420000	2.8581120000
H	-32.9103290000	-4.8662330000	1.3423200000
H	-36.3527950000	-5.9948900000	2.5896600000
H	-34.7435940000	-6.5630180000	2.1501980000
H	-36.3767560000	-7.1016180000	0.3414310000
H	-35.1689070000	-5.9424740000	-0.2684770000
H	-36.7973190000	-5.3796840000	0.1665570000
H	-36.6911360000	-1.7286500000	4.7642110000
H	-39.2886930000	-1.8370600000	5.2143970000
H	-40.4831000000	-3.5670950000	3.6008220000
H	31.2423520000	-0.4491350000	1.0404440000
H	33.2798060000	-1.9837050000	0.4366420000
H	31.3384590000	-6.2952830000	-0.8382330000
H	32.5002390000	-8.6470970000	-0.9514150000

H 34.1805540000 -8.7870030000 -1.4629070000
H 32.6253580000 -9.5158570000 -3.2876680000
H 33.5268270000 -8.0711630000 -3.8094900000
H 31.8357860000 -7.9187670000 -3.2857100000
H 37.2011600000 -5.2907920000 -0.1702720000
H 39.3839140000 -6.4232420000 -1.1264620000
H 38.8088560000 -8.2406580000 -2.9674710000

Vibrational Frequencies(cm^-1)
[1.0837000e+00 1.3773000e+00 1.9421000e+00 2.5698000e+00 3.4363000e+00
4.3940000e+00 4.4714000e+00 6.1484000e+00 6.7941000e+00 7.9036000e+00
8.3046000e+00 8.6723000e+00 9.0354000e+00 9.6036000e+00 1.1821700e+01
1.3275200e+01 1.4590500e+01 1.5831800e+01 1.7506800e+01 1.8606200e+01
2.1421300e+01 2.3708300e+01 2.4700100e+01 2.5266100e+01 2.7197200e+01
2.8089800e+01 2.8597200e+01 2.9463400e+01 3.1261700e+01 3.3356900e+01
3.4717600e+01 3.5263800e+01 3.6947700e+01 4.1069300e+01 4.1295400e+01
4.1595300e+01 4.2522300e+01 4.4397900e+01 4.6406500e+01 4.7832500e+01
4.8063900e+01 4.8157400e+01 4.8949100e+01 5.2366900e+01 5.4174200e+01
5.6588800e+01 5.8637100e+01 6.3807300e+01 6.6023300e+01 7.1663600e+01
7.2584300e+01 7.3256900e+01 7.4993200e+01 7.5908000e+01 7.7884000e+01
7.8958200e+01 8.0662300e+01 8.1130000e+01 8.3308700e+01 8.6642800e+01
8.9528300e+01 9.0736900e+01 9.1493100e+01 9.5020900e+01 9.5974100e+01
9.9158000e+01 1.0443060e+02 1.0887810e+02 1.1876740e+02 1.2000820e+02
1.2138310e+02 1.2213940e+02 1.2351970e+02 1.2523480e+02 1.2604660e+02
1.2797720e+02 1.3157400e+02 1.3510030e+02 1.3739220e+02 1.4008030e+02
1.4492850e+02 1.4690930e+02 1.4791330e+02 1.4952150e+02 1.5168440e+02
1.6122740e+02 1.6681120e+02 1.6848290e+02 1.7012690e+02 1.7203640e+02
1.7762050e+02 1.8057200e+02 1.8413630e+02 1.9690280e+02 1.9984050e+02
2.0113200e+02 2.0271560e+02 2.0570670e+02 2.0774310e+02 2.1083150e+02
2.1172820e+02 2.1289530e+02 2.1467550e+02 2.1714630e+02 2.1958440e+02
2.2050080e+02 2.2490190e+02 2.2681920e+02 2.2810310e+02 2.3131850e+02
2.3779030e+02 2.4025600e+02 2.4143380e+02 2.4547240e+02 2.5309220e+02
2.5470120e+02 2.5705080e+02 2.5780270e+02 2.6467290e+02 2.7204320e+02
2.7372120e+02 2.7706610e+02 2.7889140e+02 2.8051540e+02 2.8353790e+02
2.8650350e+02 2.9251660e+02 2.9469990e+02 2.9670550e+02 2.9742140e+02
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3.1701930e+02 3.2210940e+02 3.2265450e+02 3.2802670e+02 3.2933140e+02

3.3232890e+02 3.3528860e+02 3.4439300e+02 3.4837800e+02 3.5126260e+02
3.5450880e+02 3.5681300e+02 3.6054170e+02 3.6905510e+02 3.7055200e+02
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3.8167150e+02 3.8183810e+02 3.8927280e+02 3.9395660e+02 3.9935700e+02
4.1283890e+02 4.1502270e+02 4.2118520e+02 4.2170190e+02 4.2262940e+02
4.2632250e+02 4.3418180e+02 4.3791250e+02 4.3823860e+02 4.4028660e+02
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5.7858100e+02 5.7938150e+02 5.8442920e+02 5.8521060e+02 5.8659540e+02
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6.7842400e+02 6.9547630e+02 6.9556330e+02 6.9700930e+02 6.9721830e+02
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7.0575830e+02 7.2388360e+02 7.2417690e+02 7.2647190e+02 7.2736850e+02
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9.3974290e+02 9.4788490e+02 9.4843150e+02 9.5240400e+02 9.5591550e+02
9.5609930e+02 9.6730810e+02 9.7245530e+02 9.7439340e+02 1.0137079e+03
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1.0235385e+03 1.0236771e+03 1.0240234e+03 1.0252390e+03 1.0255830e+03
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1.0705347e+03 1.0709714e+03 1.0715796e+03 1.0717066e+03 1.0786263e+03
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1.2417315e+03 1.2447065e+03 1.2447685e+03 1.2507809e+03 1.2513931e+03
1.2516673e+03 1.2558705e+03 1.2569302e+03 1.2608365e+03 1.2622154e+03
1.2633059e+03 1.2658577e+03 1.2663742e+03 1.2667289e+03 1.2683355e+03
1.2703535e+03 1.2706352e+03 1.2763762e+03 1.2765035e+03 1.2875190e+03
1.2894924e+03 1.2960914e+03 1.2975546e+03 1.3042886e+03 1.3075098e+03
1.3111627e+03 1.3167890e+03 1.3203064e+03 1.3250445e+03 1.3312353e+03
1.3351012e+03 1.3417270e+03 1.3427326e+03 1.3435911e+03 1.3445320e+03
1.3505504e+03 1.3506128e+03 1.3621422e+03 1.3638812e+03 1.3641754e+03
1.3763182e+03 1.3766257e+03 1.3773471e+03 1.3786693e+03 1.3787202e+03
1.3798093e+03 1.3803225e+03 1.3804622e+03 1.3819610e+03 1.3838764e+03
1.3864222e+03 1.3896599e+03 1.3909749e+03 1.3962481e+03 1.3963615e+03
1.3964586e+03 1.3968660e+03 1.3969115e+03 1.3970033e+03 1.4028418e+03
1.4028928e+03 1.4029489e+03 1.4207599e+03 1.4214039e+03 1.4249113e+03
1.4257327e+03 1.4286493e+03 1.4287951e+03 1.4292347e+03 1.4310379e+03
1.4314965e+03 1.4408738e+03 1.4410754e+03 1.4438620e+03 1.4587473e+03
1.4592022e+03 1.4593662e+03 1.4641645e+03 1.4642773e+03 1.4647658e+03
1.4647897e+03 1.4650641e+03 1.4651031e+03 1.4660574e+03 1.4661653e+03

1.4661799e+03 1.4665237e+03 1.4682187e+03 1.4682419e+03 1.4683484e+03
1.4683788e+03 1.4684068e+03 1.4684487e+03 1.4733724e+03 1.4739061e+03
1.4771060e+03 1.4774721e+03 1.4780469e+03 1.4782529e+03 1.4782610e+03
1.4797147e+03 1.4802563e+03 1.4820402e+03 1.4821140e+03 1.4842288e+03
1.4844619e+03 1.4872223e+03 1.4874535e+03 1.4893306e+03 1.4894431e+03
1.4901784e+03 1.4903133e+03 1.4906024e+03 1.4949615e+03 1.4954925e+03
1.4987606e+03 1.4989756e+03 1.4994071e+03 1.5001365e+03 1.5015271e+03
1.5033364e+03 1.5039976e+03 1.5380940e+03 1.5392144e+03 1.5451920e+03
1.5508023e+03 1.5527545e+03 1.5548825e+03 1.5622184e+03 1.5690117e+03
1.5709761e+03 1.5798732e+03 1.5814205e+03 1.5826714e+03 1.5900864e+03
1.5931367e+03 1.5956710e+03 1.6062211e+03 1.6065582e+03 1.6106708e+03
1.6120014e+03 1.6126447e+03 1.6128456e+03 1.6406615e+03 1.6407774e+03
1.6451299e+03 1.7946422e+03 1.7948718e+03 1.8005445e+03 1.8394808e+03
1.8396442e+03 1.8455414e+03 3.0302685e+03 3.0305813e+03 3.0305917e+03
3.0306261e+03 3.0307034e+03 3.0308517e+03 3.0385153e+03 3.0385414e+03
3.0385899e+03 3.0387840e+03 3.0387901e+03 3.0398963e+03 3.0399880e+03
3.0401350e+03 3.0402468e+03 3.0725943e+03 3.0741046e+03 3.0743181e+03
3.0885243e+03 3.0888186e+03 3.0893077e+03 3.0895525e+03 3.0896522e+03
3.0902412e+03 3.1136570e+03 3.1140929e+03 3.1141054e+03 3.1142379e+03
3.1142483e+03 3.1144269e+03 3.1190133e+03 3.1193150e+03 3.1193314e+03
3.1194990e+03 3.1195029e+03 3.1196634e+03 3.1216710e+03 3.1226042e+03
3.1226847e+03 3.1249868e+03 3.1253059e+03 3.1253078e+03 3.1407185e+03
3.1417477e+03 3.1418387e+03 3.1430459e+03 3.1433317e+03 3.1641494e+03
3.1967333e+03 3.1971491e+03 3.1977229e+03 3.1978807e+03 3.1983324e+03
3.1985268e+03 3.2046361e+03 3.2046548e+03 3.2046968e+03 3.2049962e+03
3.2060812e+03 3.2065125e+03 3.2073993e+03 3.2075279e+03 3.2076785e+03
3.2083386e+03 3.2099685e+03 3.2100867e+03 3.2182652e+03 3.2183909e+03
3.2184594e+03 3.2185594e+03 3.2187879e+03 3.2191450e+03 3.2255494e+03
3.2493982e+03 3.2496608e+03 3.2503676e+03 3.2512360e+03 3.2512818e+03
3.2527940e+03 3.2537555e+03]

Calculations for **P5**:

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[Geometry 77]

O -27.4491950000 0.2437610000 -0.0525580000

C -26.2809260000 -0.0698900000 -0.1200950000

N -25.8368400000 -1.3697160000 -0.3697330000

C	-26.7279690000	-2.4991560000	-0.6033350000
C	-27.0603820000	-2.7088250000	-2.0801240000
C	-24.4492660000	-1.4611080000	-0.3977090000
C	-23.9298110000	-0.0714070000	-0.1289820000
C	-22.6217660000	0.4388320000	-0.0251920000
C	-21.3488650000	-0.2654910000	-0.1519340000
C	-21.0623300000	-1.5866590000	-0.4671710000
C	-19.6813580000	-1.8816470000	-0.4955770000
C	-18.8689290000	-0.7974020000	-0.2011090000
C	-17.4247490000	-0.7407150000	-0.1387960000
C	-16.6205760000	0.3481780000	0.1060480000
C	-15.2215620000	0.0463120000	0.0911620000
C	-14.1335330000	0.9238270000	0.2897820000
O	-14.3448740000	2.2520030000	0.5308680000
C	-14.3359040000	2.6582560000	1.9072620000
C	-14.5490740000	4.1568770000	1.9607520000
C	-12.8483810000	0.3909530000	0.1865430000
S	-11.3465820000	1.2837590000	0.3372270000
C	-10.3999700000	-0.1858480000	0.0425080000
C	-8.9542870000	-0.1163480000	0.0312960000
C	-8.1481220000	1.0133550000	0.0951000000
C	-6.7753560000	0.7112470000	0.0548280000
C	-6.4964150000	-0.6508650000	-0.0374810000
C	-5.1280470000	-1.1687860000	-0.0958220000
C	-4.6749990000	-2.4982580000	-0.1855360000
C	-3.2956430000	-2.8071760000	-0.2359430000
C	-3.1827830000	-4.3078010000	-0.3305580000
N	-4.4854690000	-4.7966820000	-0.3314100000
C	-4.8182360000	-6.2143440000	-0.3948970000
C	-4.8738170000	-6.8821830000	0.9784880000
C	-5.4362390000	-3.7790340000	-0.2446790000
O	-6.6330620000	-3.9704010000	-0.2280490000
O	-2.2045000000	-5.0222330000	-0.3991220000
C	-2.3211590000	-1.7913080000	-0.1963280000
C	-0.8674600000	-1.9120510000	-0.2368500000
C	-0.0450320000	-3.0267870000	-0.3329410000
C	1.3335550000	-2.7216530000	-0.3432950000

C	1.6098440000	-1.3654860000	-0.2562290000
C	2.8965490000	-0.7049870000	-0.2413030000
C	3.1666880000	0.6433380000	-0.2036680000
C	4.5643840000	0.9513180000	-0.2012830000
C	5.1809770000	2.2209630000	-0.1629920000
O	4.4270970000	3.3598880000	-0.1371730000
C	4.1914990000	3.9392600000	1.1551760000
C	3.3770690000	5.2022790000	0.9669080000
C	6.5753390000	2.2610490000	-0.1825870000
S	7.5665980000	3.7076150000	-0.1699930000
C	9.0497910000	2.7368470000	-0.1996750000
C	10.3388380000	3.3947330000	-0.1902000000
C	10.6019180000	4.7593770000	-0.1858530000
C	11.9786190000	5.0694740000	-0.1788090000
C	12.7915350000	3.9441400000	-0.1772400000
C	14.2359590000	3.7592220000	-0.1688820000
C	15.2569830000	4.7313850000	-0.1659640000
C	16.6193690000	4.3511150000	-0.1513180000
C	17.4338580000	5.6195880000	-0.1470360000
N	16.5204280000	6.6680670000	-0.1461780000
C	16.9042030000	8.0744600000	-0.1621430000
C	17.0866270000	8.6330810000	-1.5727620000
C	15.1963580000	6.2269480000	-0.1639290000
O	14.2451290000	6.9795220000	-0.1714220000
O	18.6357540000	5.7842590000	-0.1469180000
C	17.0027590000	2.9942700000	-0.1320730000
C	18.3449650000	2.4204610000	-0.0962340000
C	19.5978070000	3.0116460000	-0.1865560000
C	20.6698780000	2.0946430000	-0.1180300000
C	20.2721390000	0.7749770000	0.0313590000
C	21.0947090000	-0.4107000000	0.1397550000
C	20.6955410000	-1.7210190000	0.2546580000
C	21.7830680000	-2.6497700000	0.3422670000
C	21.7269570000	-4.0525320000	0.4740360000
O	20.5249070000	-4.7001270000	0.5171440000
C	20.0148440000	-5.0125630000	1.8220640000
C	18.7066090000	-5.7570830000	1.6539140000

C	22.9394910000	-4.7449300000	0.5282570000
S	23.1348650000	-6.4849300000	0.6652190000
C	24.8754470000	-6.3140350000	0.6590440000
C	25.2965120000	-5.0236640000	0.5466330000
C	24.2046670000	-4.0873300000	0.4598300000
C	24.2597180000	-2.6843670000	0.3275470000
O	25.4582070000	-2.0280910000	0.2824490000
C	25.9934800000	-1.7754430000	-1.0245690000
C	27.2935370000	-1.0144700000	-0.8657910000
C	23.0490760000	-1.9933420000	0.2733110000
S	22.8608560000	-0.2546060000	0.1378260000
S	18.5328870000	0.6740640000	0.0881900000
C	15.8797100000	2.1061790000	-0.1494470000
N	14.6174260000	2.4538130000	-0.1657270000
S	11.8227050000	2.4782310000	-0.1840220000
C	8.7776260000	1.3887910000	-0.2320040000
C	7.3797260000	1.0815810000	-0.2331510000
C	6.7627310000	-0.1878970000	-0.2728430000
O	7.5109780000	-1.3304810000	-0.3004160000
C	7.7940960000	-1.8737300000	-1.5990110000
C	8.6003630000	-3.1427800000	-1.4164120000
C	5.3688170000	-0.2274600000	-0.2544590000
S	4.3795270000	-1.6755530000	-0.2707430000
S	0.1266890000	-0.4546860000	-0.1562590000
C	-2.9003120000	-0.4833550000	-0.1011220000
N	-4.1760650000	-0.1964340000	-0.0550940000
S	-7.9918640000	-1.5676130000	-0.0695940000
C	-11.2062740000	-1.2813970000	-0.1628000000
C	-12.6056530000	-0.9903890000	-0.0851900000
C	-13.6944590000	-1.8718700000	-0.2625450000
O	-13.4915360000	-3.1927240000	-0.5456350000
C	-13.4428740000	-4.0832990000	0.5789240000
C	-13.2382540000	-5.4914660000	0.0600540000
C	-14.9785500000	-1.3341950000	-0.1818520000
S	-16.4777470000	-2.2135540000	-0.4143830000
S	-19.8417080000	0.6136970000	0.1185140000
C	-22.6053410000	1.8459750000	0.2422020000

N	-23.6475360000	2.6236100000	0.3937230000
C	-24.9167520000	2.1418810000	0.3053340000
C	-25.9486910000	3.1650850000	0.5094480000
C	-25.6362300000	4.4970140000	0.7648740000
C	-26.7686400000	5.3275880000	0.9328230000
C	-27.9462510000	4.6266240000	0.8052330000
S	-27.6917940000	2.9559530000	0.4805090000
C	-25.0565730000	0.7681920000	0.0358820000
O	-23.8545820000	-2.4983330000	-0.6051710000
H	-27.6427880000	-2.3043430000	-0.0251550000
H	-26.2330590000	-3.3895960000	-0.1890320000
H	-26.1497300000	-2.9093860000	-2.6650280000
H	-27.7350930000	-3.5718930000	-2.1940380000
H	-27.5643910000	-1.8251490000	-2.5007100000
H	-21.8463920000	-2.3129460000	-0.6669320000
H	-19.2861050000	-2.8711450000	-0.7304130000
H	-17.0055930000	1.3539320000	0.2762730000
H	-15.1339490000	2.1217630000	2.4533760000
H	-13.3719200000	2.3795850000	2.3705970000
H	-15.5116610000	4.4315880000	1.5024410000
H	-13.7483570000	4.6816180000	1.4174120000
H	-14.5483930000	4.5045840000	3.0055440000
H	-8.5439720000	2.0282160000	0.1582780000
H	-5.9745870000	1.4472040000	0.0869250000
H	-4.0572080000	-6.6948360000	-1.0269210000
H	-5.7919940000	-6.2876220000	-0.9003870000
H	-5.1296700000	-7.9476850000	0.8674720000
H	-3.9005190000	-6.8175020000	1.4884950000
H	-5.6393850000	-6.4128500000	1.6152720000
H	-0.4481560000	-4.0347060000	-0.3944550000
H	2.1134350000	-3.4811710000	-0.4164750000
H	2.3931820000	1.4116390000	-0.1912010000
H	5.1572130000	4.1610730000	1.6444720000
H	3.6567150000	3.2101180000	1.7916440000
H	3.1762570000	5.6743730000	1.9412100000
H	2.4139180000	4.9783430000	0.4828440000
H	3.9193130000	5.9223580000	0.3351000000

H	9.8170130000	5.5175820000	-0.1899970000
H	12.3838890000	6.0785150000	-0.1751590000
H	17.8396940000	8.1568940000	0.4099060000
H	16.1157510000	8.6238940000	0.3720790000
H	17.8788730000	8.0919380000	-2.1123550000
H	17.3741990000	9.6950050000	-1.5213410000
H	16.1519360000	8.5613720000	-2.1497750000
H	19.7206340000	4.0864300000	-0.2930110000
H	21.7173680000	2.3941420000	-0.1770790000
H	19.6508870000	-2.0330750000	0.2660450000
H	20.7511140000	-5.6266310000	2.3716910000
H	19.8711570000	-4.0766350000	2.3931990000
H	17.9735160000	-5.1418600000	1.1096620000
H	18.8608230000	-6.6883550000	1.0876160000
H	18.2847500000	-6.0125860000	2.6384080000
H	25.4949880000	-7.2068830000	0.7404690000
H	26.3442790000	-4.7237140000	0.5329580000
H	25.2646740000	-1.1934540000	-1.6178160000
H	26.1549510000	-2.7359060000	-1.5482700000
H	27.7341800000	-0.8027280000	-1.8524580000
H	27.1222810000	-0.0586160000	-0.3473500000
H	28.0186470000	-1.5981960000	-0.2778790000
H	16.0632760000	1.0253440000	-0.1562700000
H	9.5518780000	0.6214030000	-0.2470560000
H	8.3523040000	-1.1285750000	-2.1953100000
H	6.8461020000	-2.0797400000	-2.1285810000
H	9.5457670000	-2.9331810000	-0.8926580000
H	8.0356270000	-3.8790010000	-0.8240920000
H	8.8355280000	-3.5883600000	-2.3955000000
H	-2.2297160000	0.3835020000	-0.0617750000
H	-10.8199290000	-2.2751080000	-0.3908630000
H	-14.3845260000	-4.0053640000	1.1527190000
H	-12.6182320000	-3.7826950000	1.2513580000
H	-13.1981470000	-6.2039520000	0.8986630000
H	-12.2970490000	-5.5659200000	-0.5060890000
H	-14.0643320000	-5.7826480000	-0.6067200000
H	-21.6353920000	2.3501770000	0.3303050000

H -24.6020030000 4.8306930000 0.8222800000
H -26.7174190000 6.3976710000 1.1390330000
H -28.9642570000 5.0079530000 0.8855870000

Vibrational Frequencies(cm^-1)
[9.9300000e-01 2.2876000e+00 3.2993000e+00 3.5438000e+00 3.7250000e+00
4.2051000e+00 4.9826000e+00 6.4324000e+00 7.0894000e+00 7.9730000e+00
9.0698000e+00 1.2740800e+01 1.3697200e+01 2.0719300e+01 2.2123500e+01
2.2574100e+01 2.3964100e+01 2.6624200e+01 2.7925300e+01 2.9267800e+01
2.9637800e+01 2.9858400e+01 3.1739100e+01 3.2319800e+01 3.3649500e+01
3.3999800e+01 3.4801300e+01 3.5453000e+01 3.7627400e+01 3.9245400e+01
4.1116300e+01 4.6835300e+01 4.6911700e+01 4.7331600e+01 4.7397600e+01
4.8615000e+01 4.8760500e+01 5.0279100e+01 5.1081700e+01 5.3100800e+01
5.3349600e+01 5.4319200e+01 5.5176700e+01 5.7676900e+01 5.8019300e+01
6.0513300e+01 6.8072800e+01 7.7734100e+01 7.7906000e+01 7.9611600e+01
8.0966400e+01 8.1576000e+01 8.5040600e+01 8.8498600e+01 9.1695100e+01
9.7551100e+01 1.0020510e+02 1.0411020e+02 1.0651470e+02 1.1281340e+02
1.1778200e+02 1.2365110e+02 1.2393920e+02 1.2415540e+02 1.2663890e+02
1.2944360e+02 1.3126980e+02 1.4124330e+02 1.4241960e+02 1.4622100e+02
1.4659520e+02 1.4734120e+02 1.6132310e+02 1.6307910e+02 1.7081380e+02
1.7781440e+02 1.7977080e+02 1.8392760e+02 1.9092210e+02 1.9160050e+02
1.9995600e+02 2.0216920e+02 2.0601950e+02 2.0704990e+02 2.0780830e+02
2.1263650e+02 2.1497300e+02 2.2085770e+02 2.2251200e+02 2.2472250e+02
2.2813630e+02 2.2923870e+02 2.3826330e+02 2.4044270e+02 2.4208850e+02
2.4385850e+02 2.4684840e+02 2.4806290e+02 2.4927210e+02 2.5323400e+02
2.5648230e+02 2.5863460e+02 2.6149730e+02 2.6459880e+02 2.6524120e+02
2.6791330e+02 2.6839070e+02 2.7334000e+02 2.7492320e+02 2.7830230e+02
2.7955080e+02 2.8044420e+02 2.8429810e+02 2.8810930e+02 2.9183240e+02
2.9404990e+02 3.0230230e+02 3.0639490e+02 3.1129970e+02 3.1796170e+02
3.2056960e+02 3.2271050e+02 3.2325740e+02 3.2458400e+02 3.2884370e+02
3.3938510e+02 3.4107780e+02 3.4405120e+02 3.4904820e+02 3.5038280e+02
3.5426400e+02 3.5616730e+02 3.5794270e+02 3.6462040e+02 3.6691810e+02
3.7361890e+02 3.7741660e+02 3.7863660e+02 3.8187280e+02 3.8727500e+02
3.8871600e+02 3.8949550e+02 3.9236980e+02 3.9795980e+02 4.0244210e+02
4.1049090e+02 4.1832360e+02 4.3550170e+02 4.4213700e+02 4.4479010e+02
4.5771180e+02 4.6571490e+02 4.7411820e+02 4.7527710e+02 4.7622420e+02
4.7825510e+02 4.8074090e+02 4.8430490e+02 4.8811850e+02 4.8913840e+02

4.9442300e+02 5.0578800e+02 5.1119290e+02 5.1591650e+02 5.1916960e+02
5.2652990e+02 5.2878720e+02 5.3000730e+02 5.3204510e+02 5.3574060e+02
5.4623650e+02 5.5660940e+02 5.5770370e+02 5.6478220e+02 5.6913380e+02
5.7794150e+02 5.8153030e+02 5.8617510e+02 5.8764460e+02 5.8862190e+02
5.9450350e+02 5.9933860e+02 6.0029370e+02 6.1276890e+02 6.1441230e+02
6.1698700e+02 6.1813570e+02 6.1839350e+02 6.2114190e+02 6.2493570e+02
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6.5243920e+02 6.5301230e+02 6.5301360e+02 6.5820560e+02 6.5888700e+02
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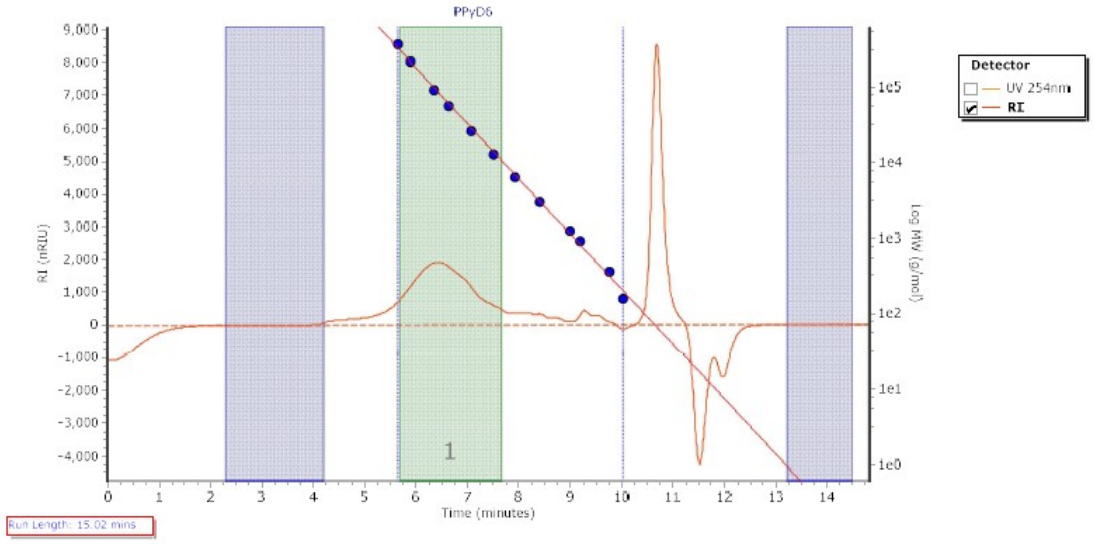
All calculations were carried out using Gaussian 16 Revision B.01

Gaussian 16, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

10. APPENDIX 2: GPC, TGA, DSC, FTIR, HR-MS and NMR spectra

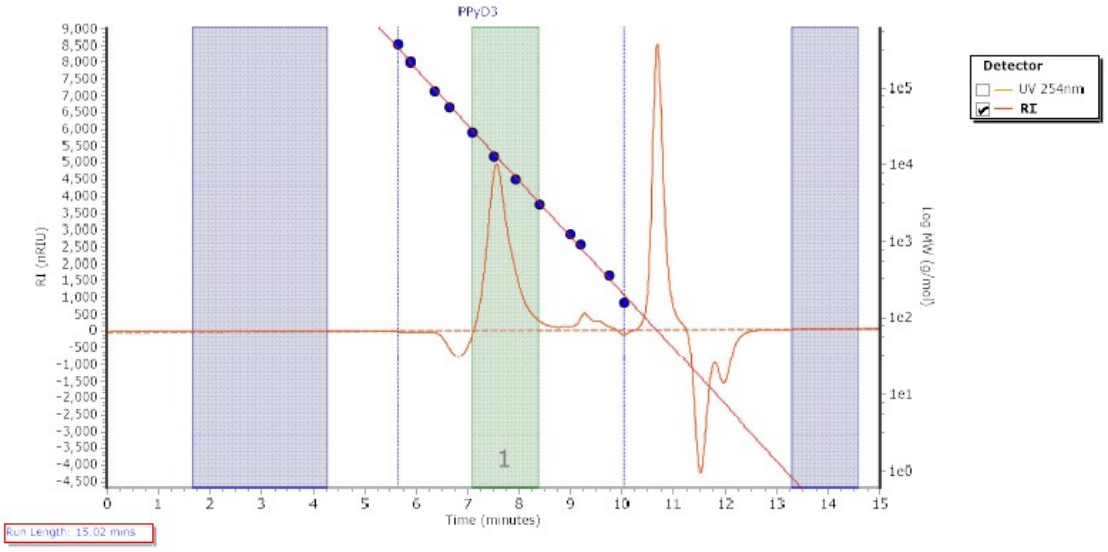
Gel permeation chromatograms of polymers **P1**:



Molecular Weight Averages

Peak	Mp (g/mol)	Mn (g/mol)	Mw (g/mol)	Mz (g/mol)	Mz+1 (g/mol)	Mv (g/mol)	PD
Peak 1	86494	47787	91672	143322	183883	136669	1.918

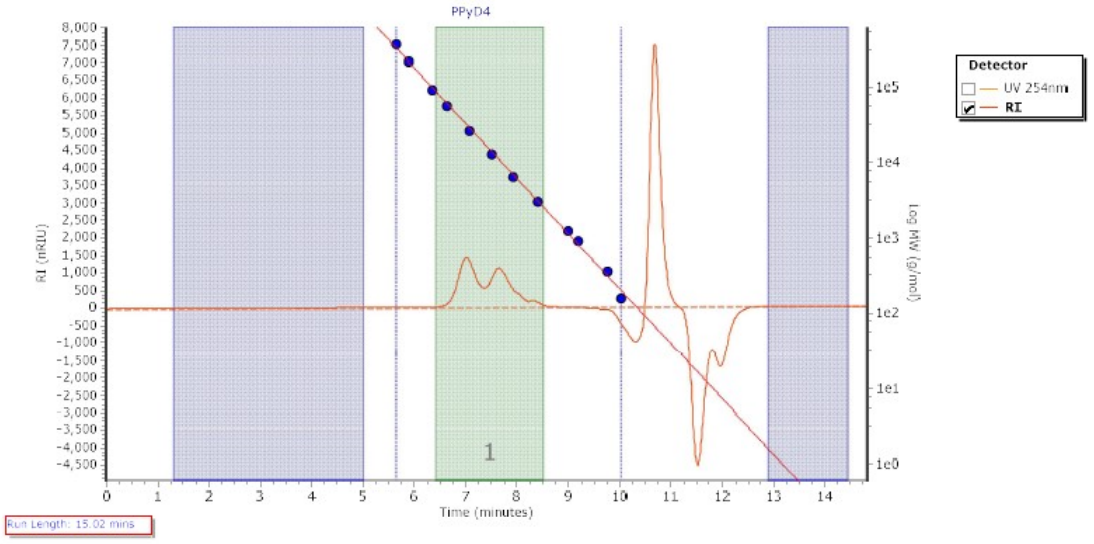
Gel permeation chromatograms of polymers **P2**:



Molecular Weight Averages

Peak	Mp (g/mol)	Mn (g/mol)	Mw (g/mol)	Mz (g/mol)	Mz+1 (g/mol)	Mv (g/mol)	PD
Peak 1	12877	10002	11806	13428	14851	13207	1.18

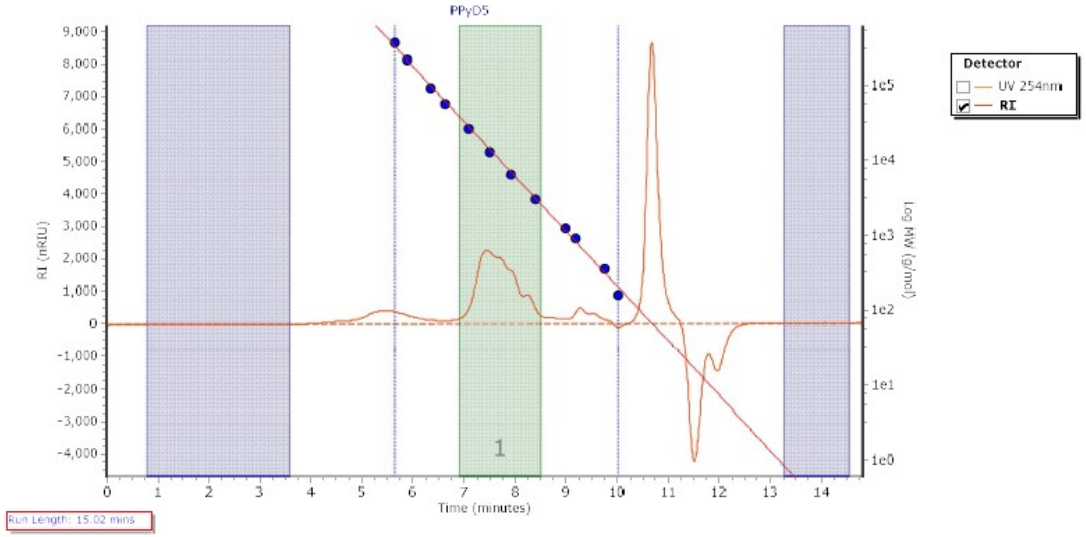
Gel permeation chromatograms of polymers **P3**:



Molecular Weight Averages

Peak	Mp (g/mol)	Mn (g/mol)	Mw (g/mol)	Mz (g/mol)	Mz+1 (g/mol)	Mv (g/mol)	PD
Peak **1**	32000	12914	21347	30149	37124	29027	1.653

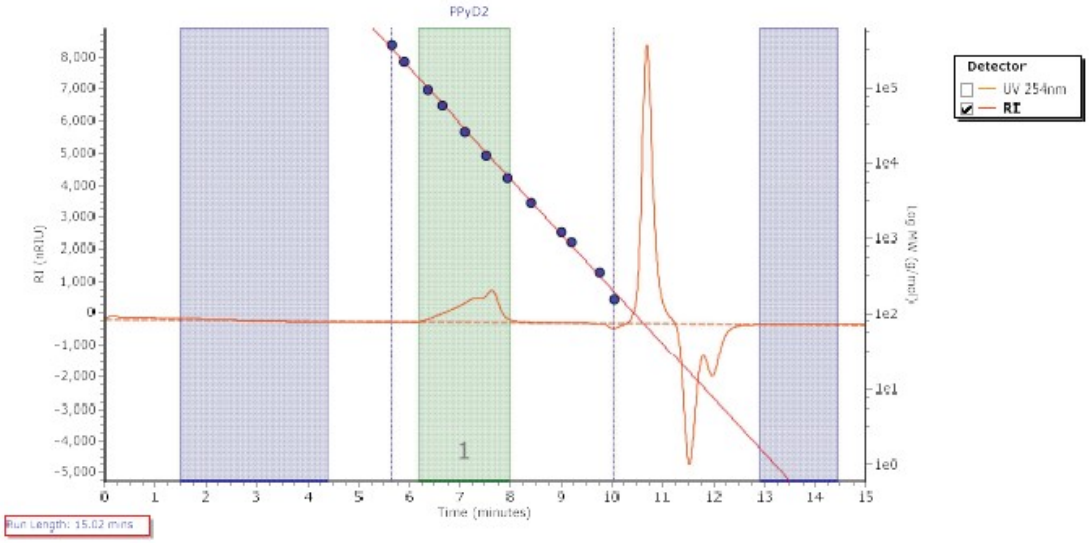
Gel permeation chromatograms of polymers **P4**:



Molecular Weight Averages

Peak	Mp (g/mol)	Mn (g/mol)	Mw (g/mol)	Mz (g/mol)	Mz+1 (g/mol)	Mv (g/mol)	PD
Peak **1**	15448	8786	12196	15822	19150	15314	1.388

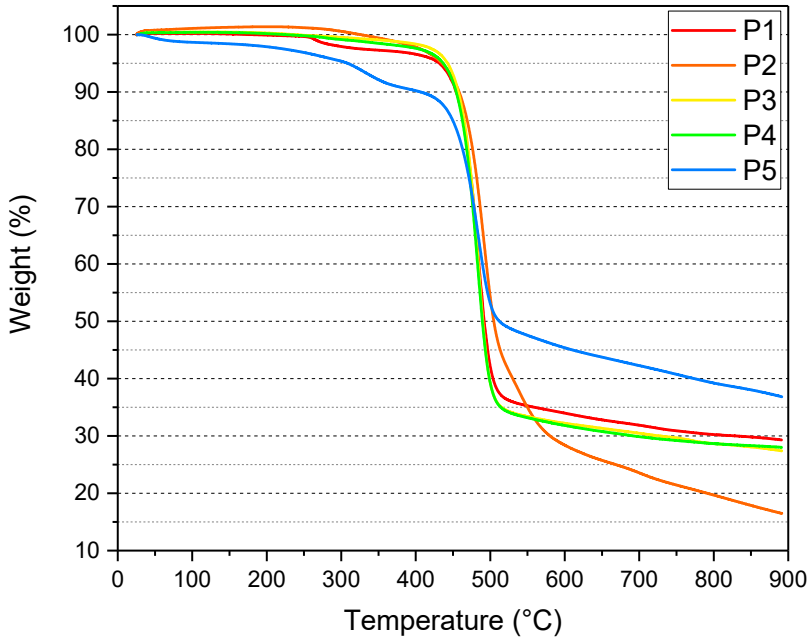
Gel permeation chromatograms of polymers **P5**:



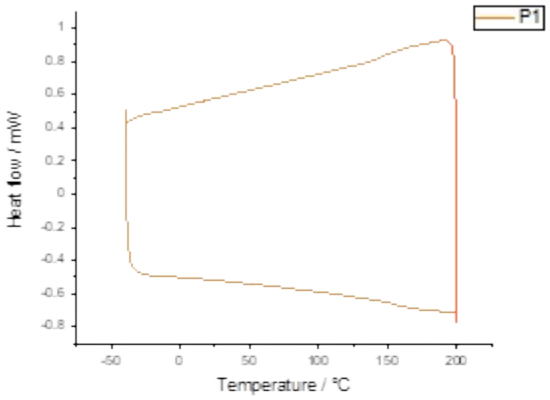
Molecular Weight Averages

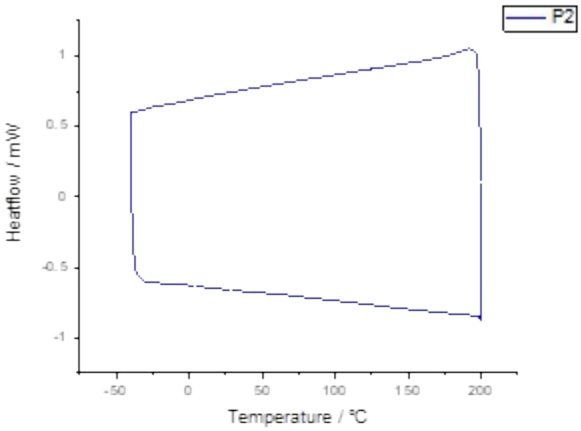
Peak	Mp (g/mol)	Mn (g/mol)	Mw (g/mol)	Mz (g/mol)	Mz+1 (g/mol)	Mv (g/mol)	PD
Peak 1	11674	17235	25234	38717	54615	36474	1.464

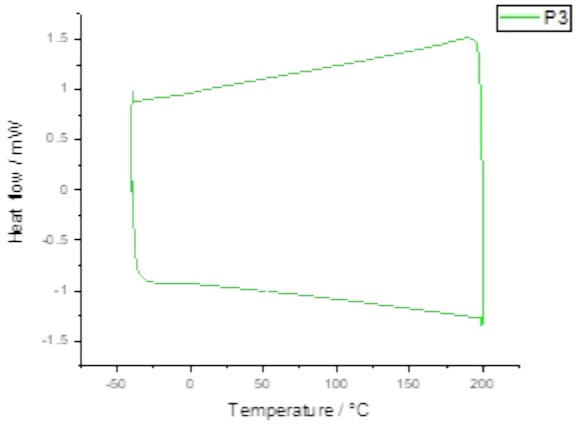
TGA Study of polymers **P1** – **P5**:

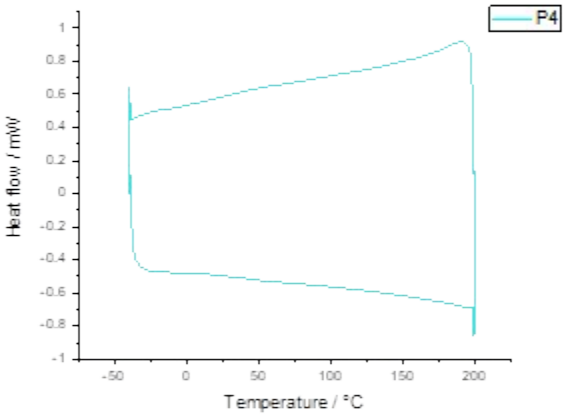


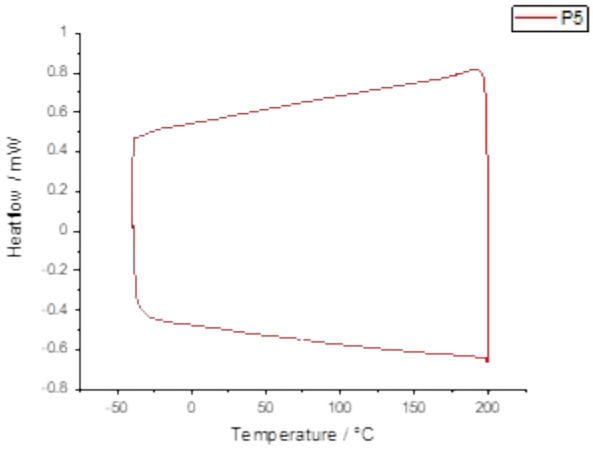
DSC Study of polymers **P1** – **P5**:



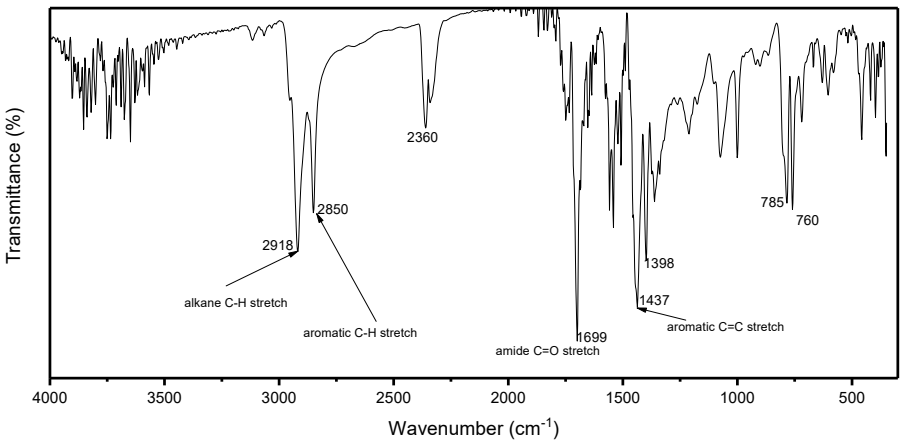




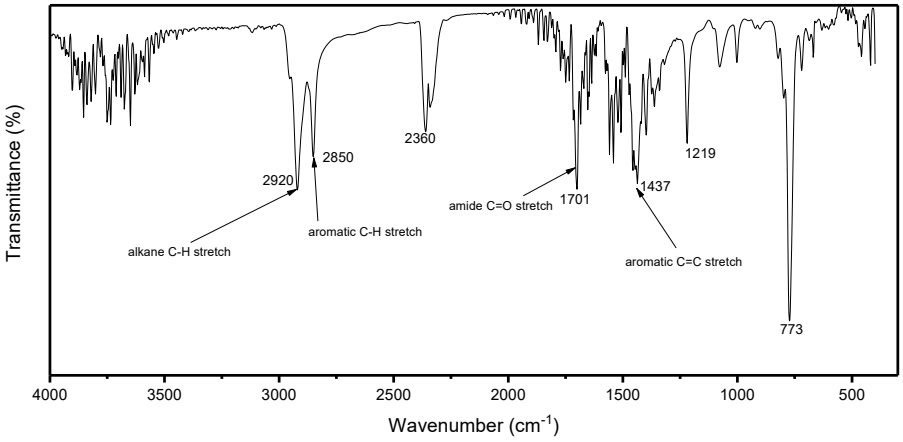




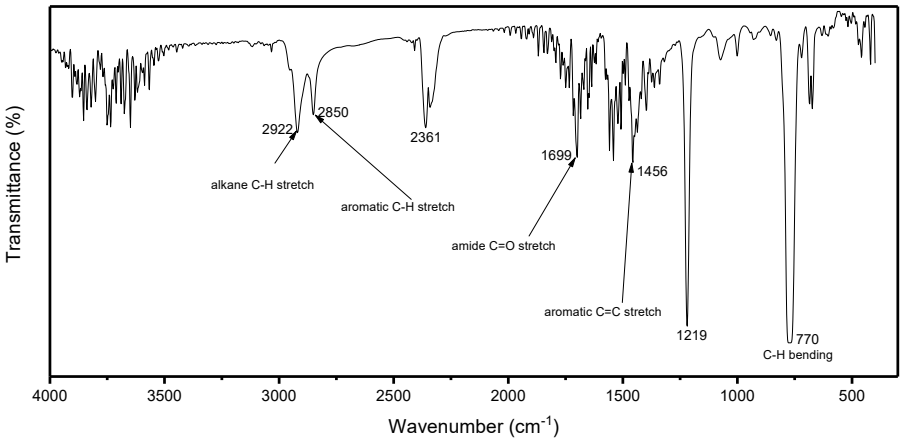
FTIR Spectra of polymer **P1**:



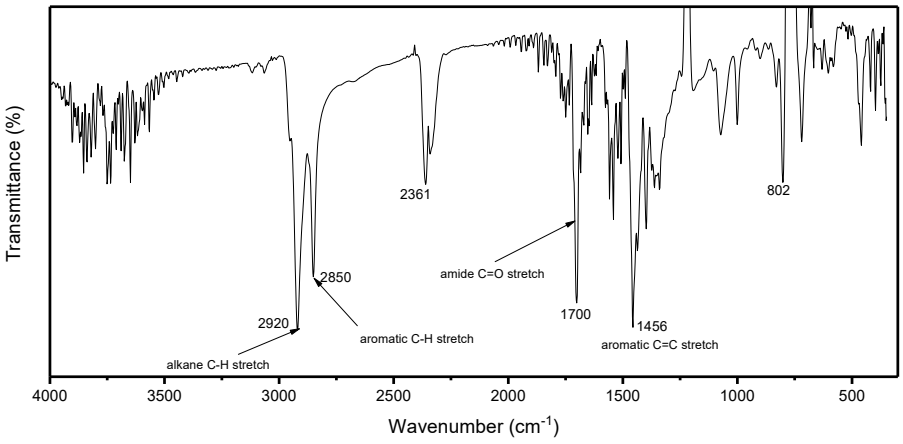
FTIR Spectra of polymer **P2**:



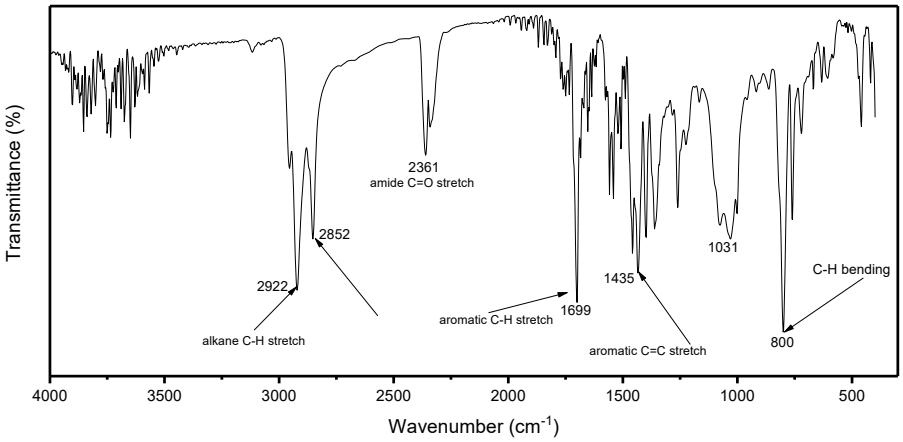
FTIR Spectra of polymer **P3**:



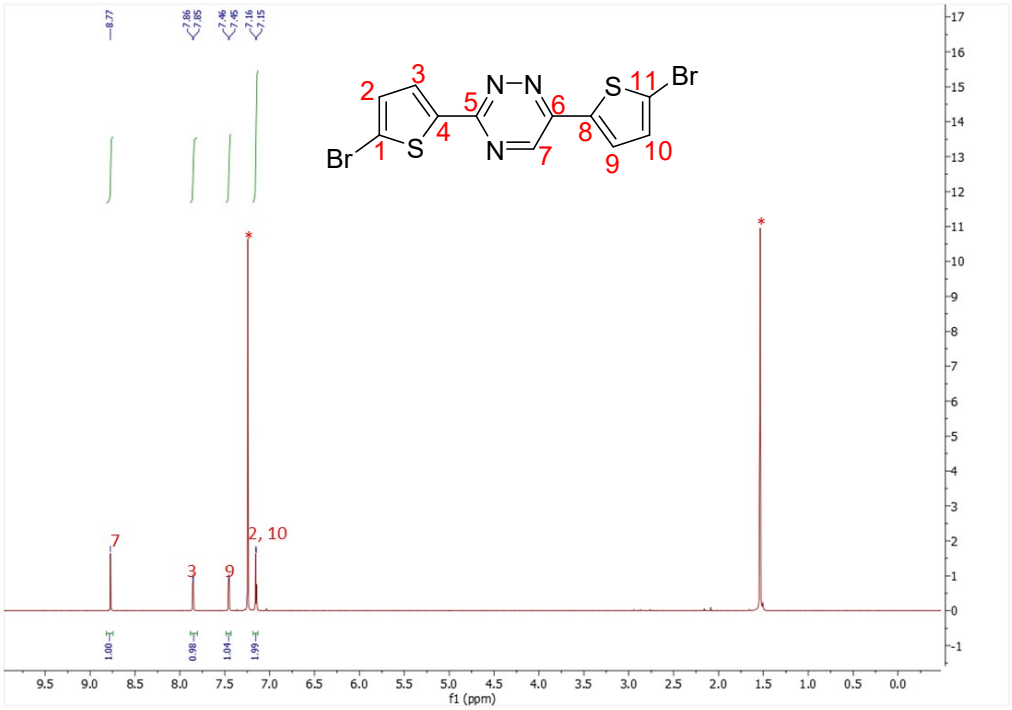
FTIR Spectra of polymer **P4**:

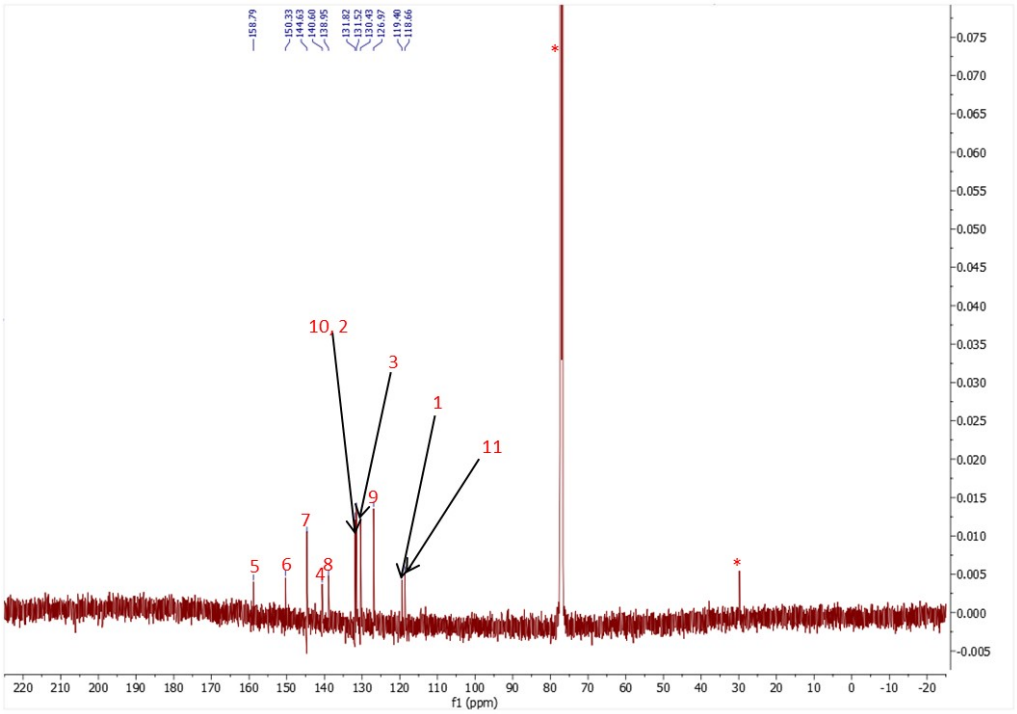


FTIR Spectra of polymer **P5**:

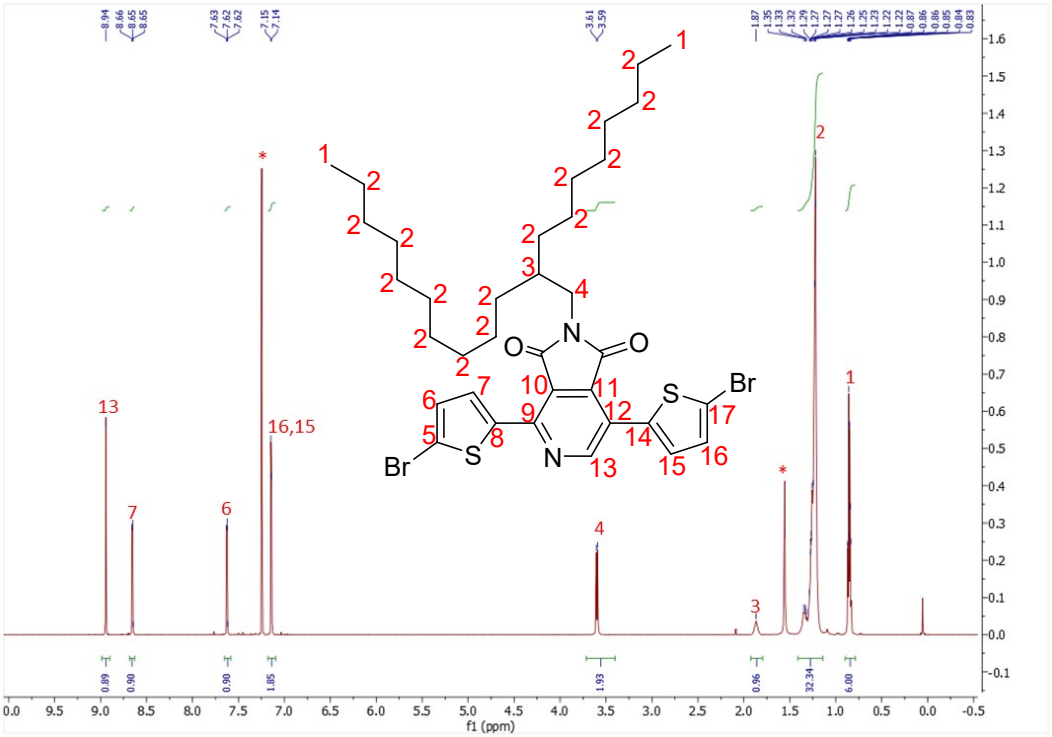


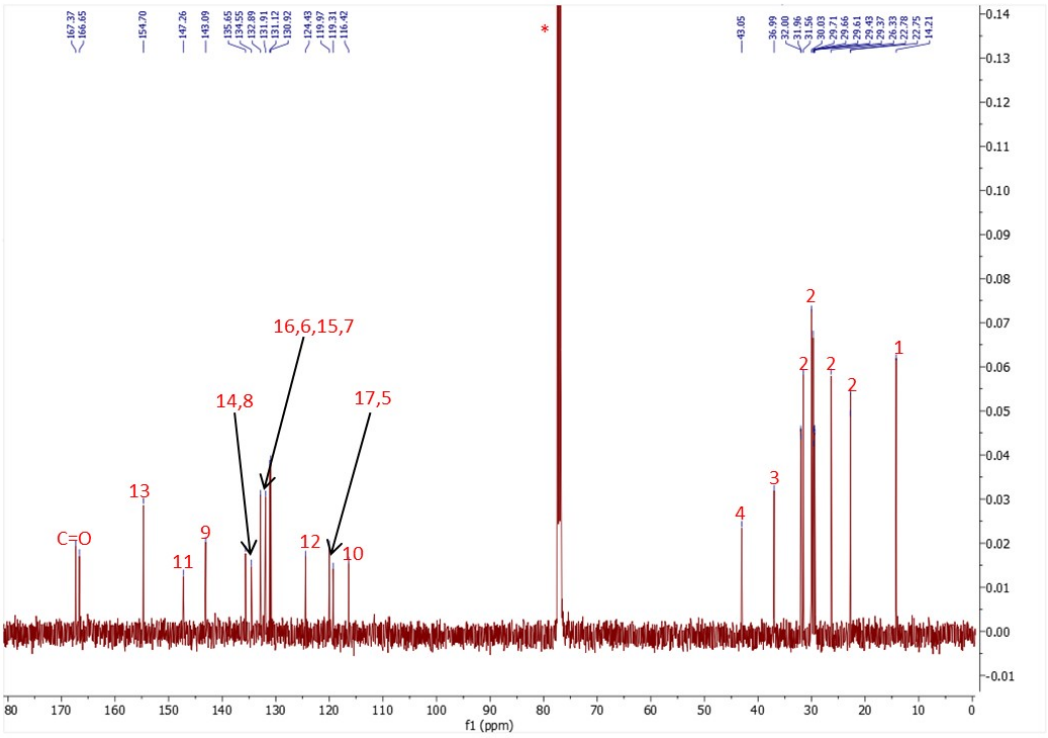
NMR Spectra of compound **7**:



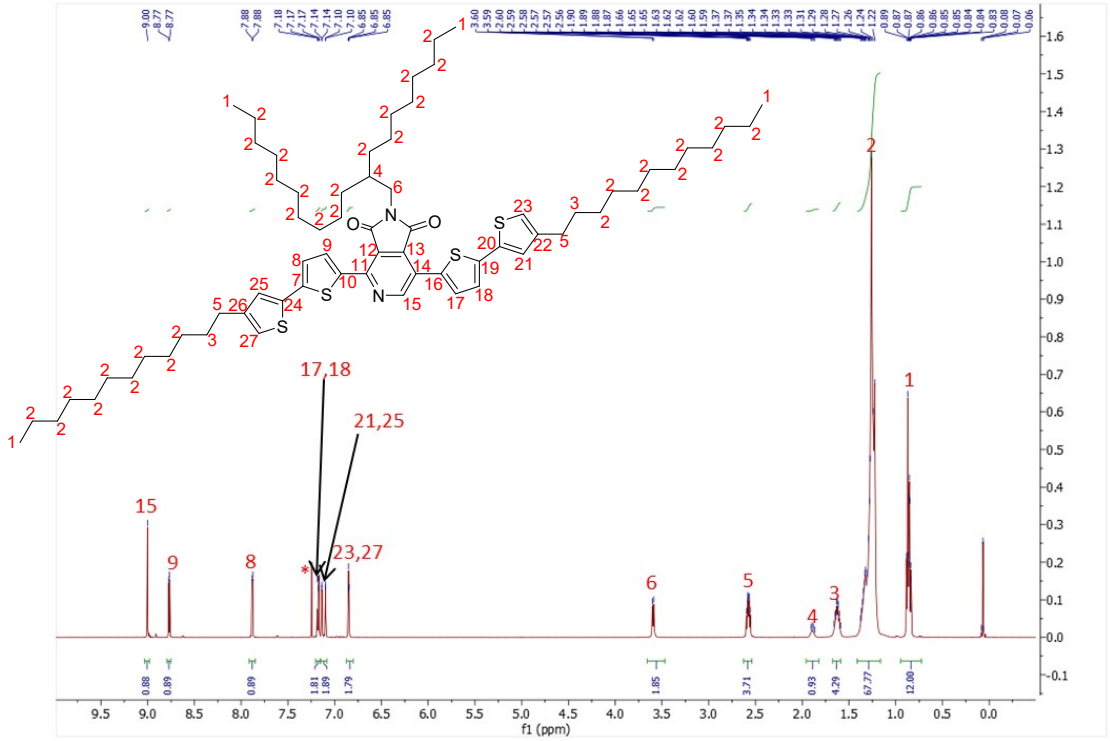


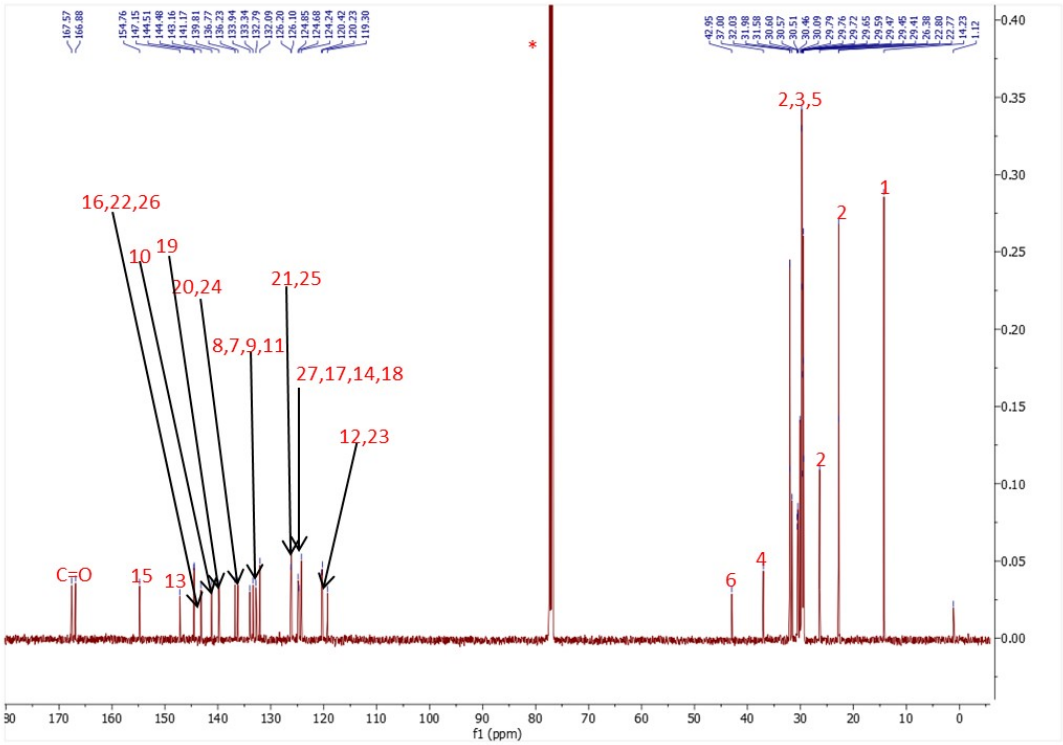
NMR Spectra of compound **8**:



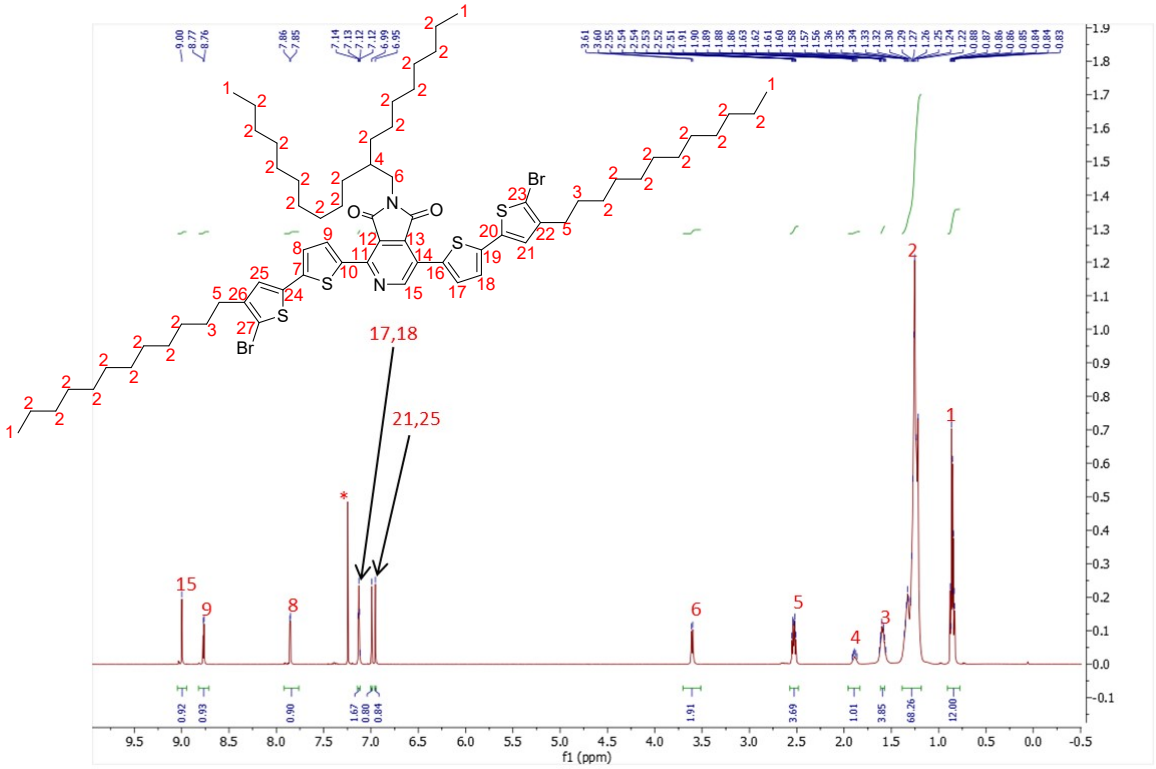


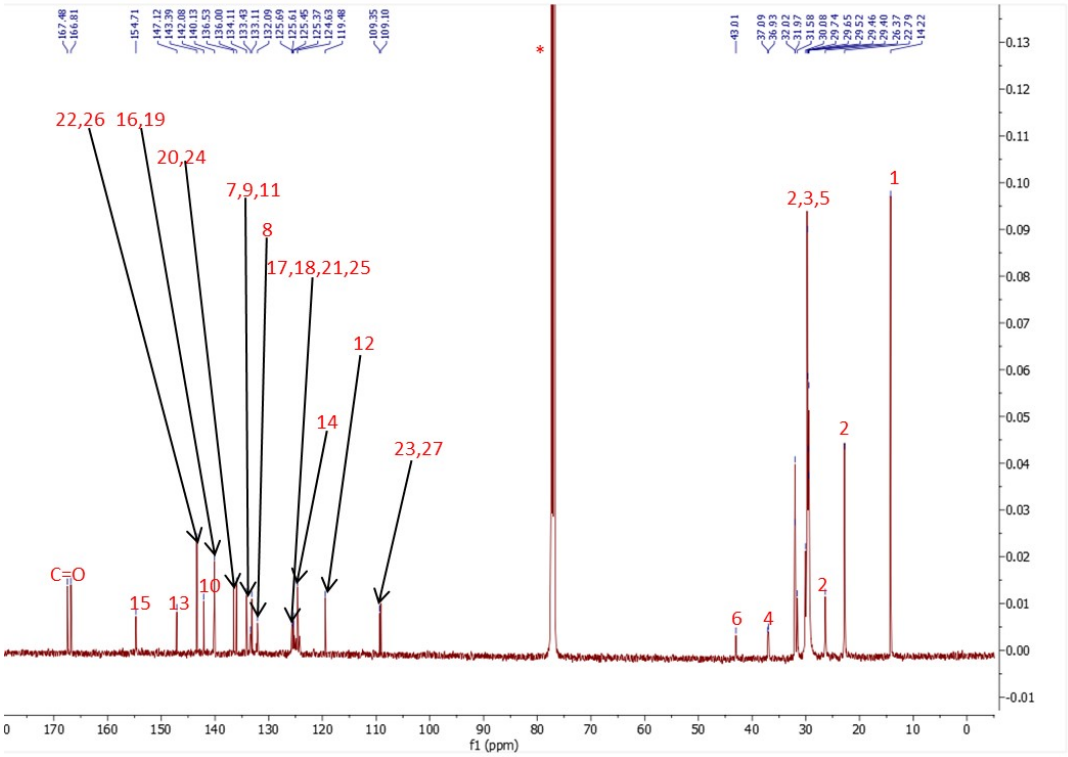
NMR Spectra of compound **9**:



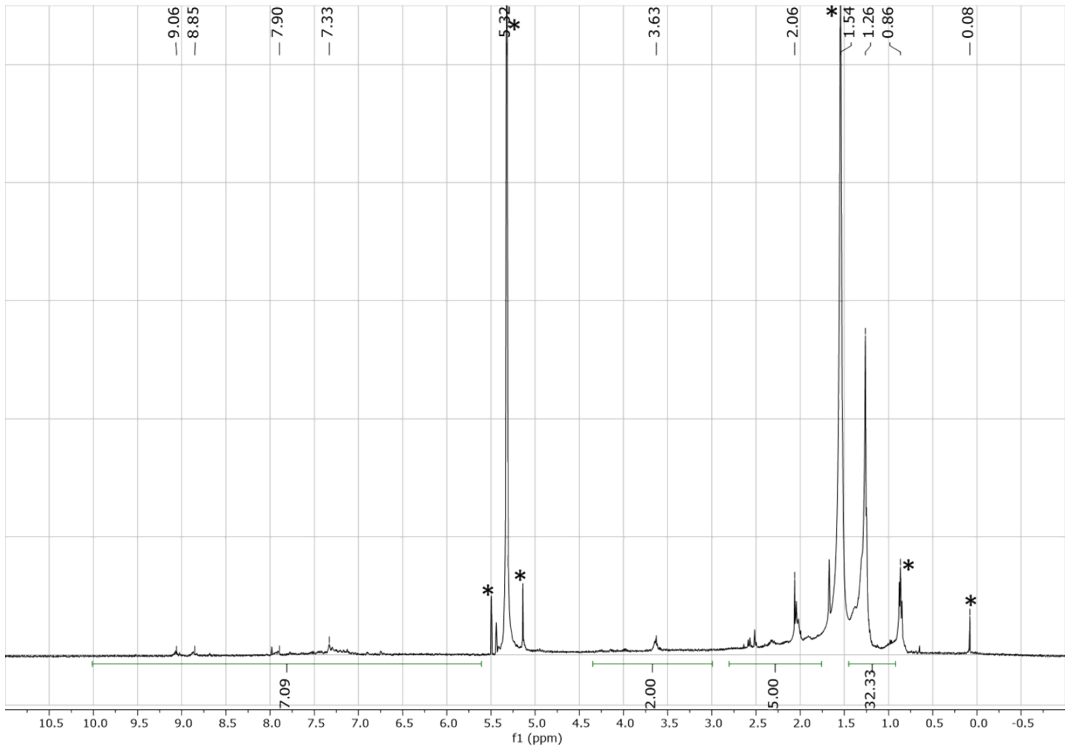


NMR Spectra of compound **10**:

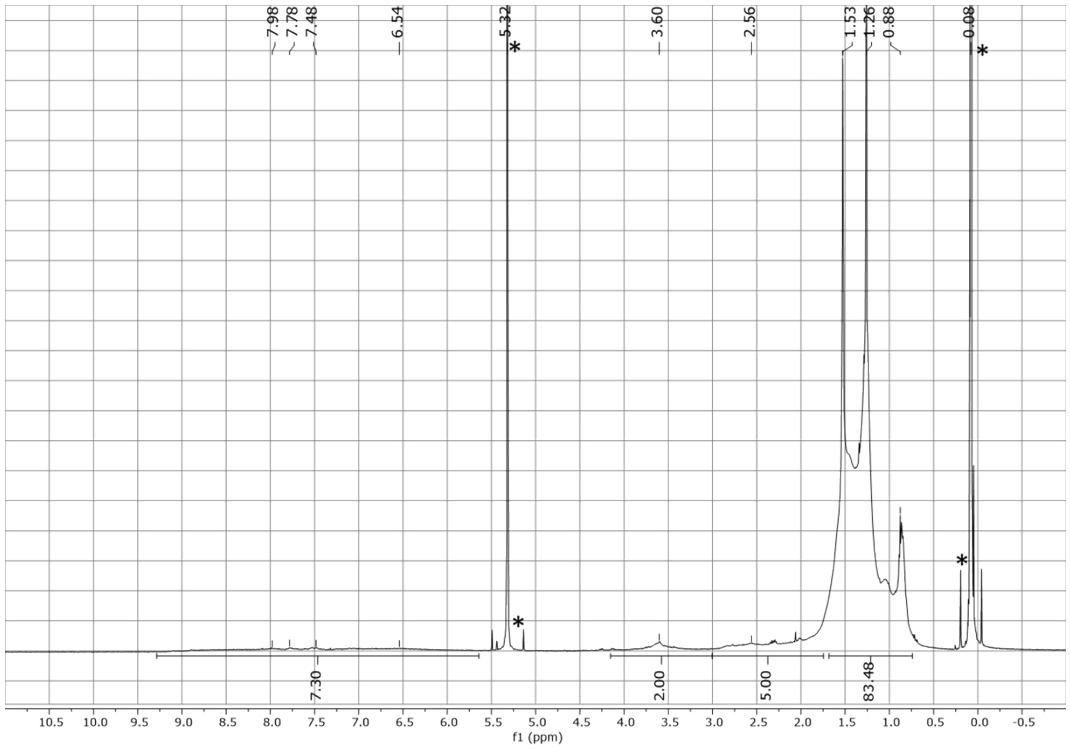




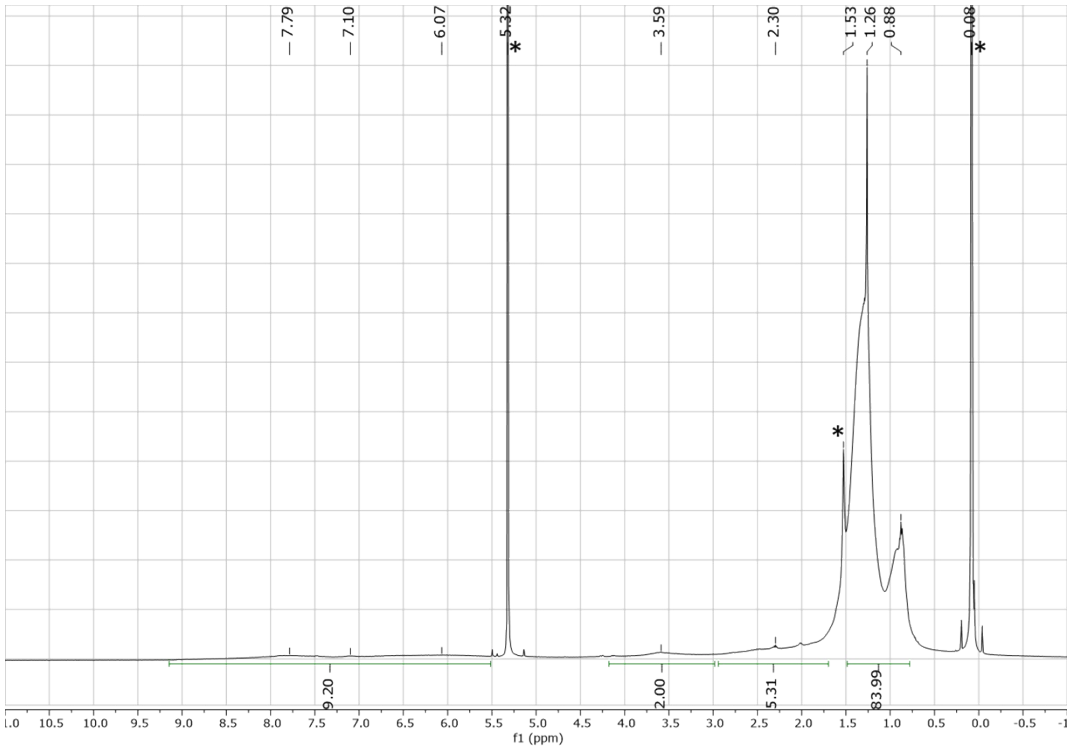
NMR Spectra of Polymer **P1**:



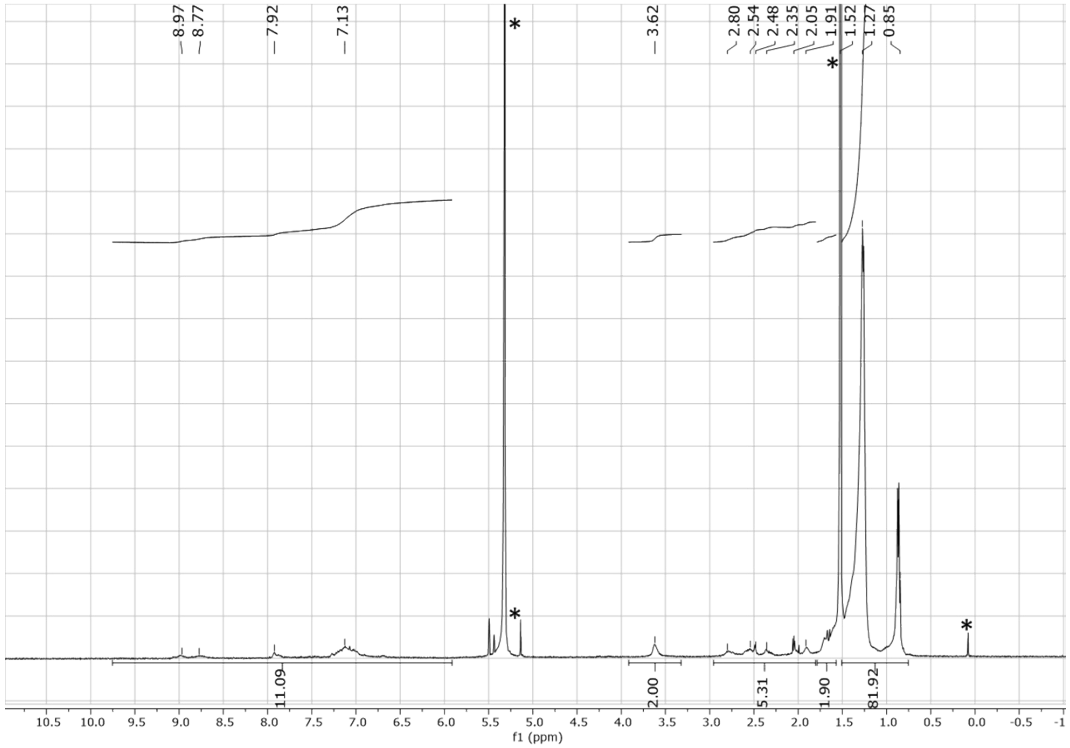
NMR Spectra of Polymer **P2**:



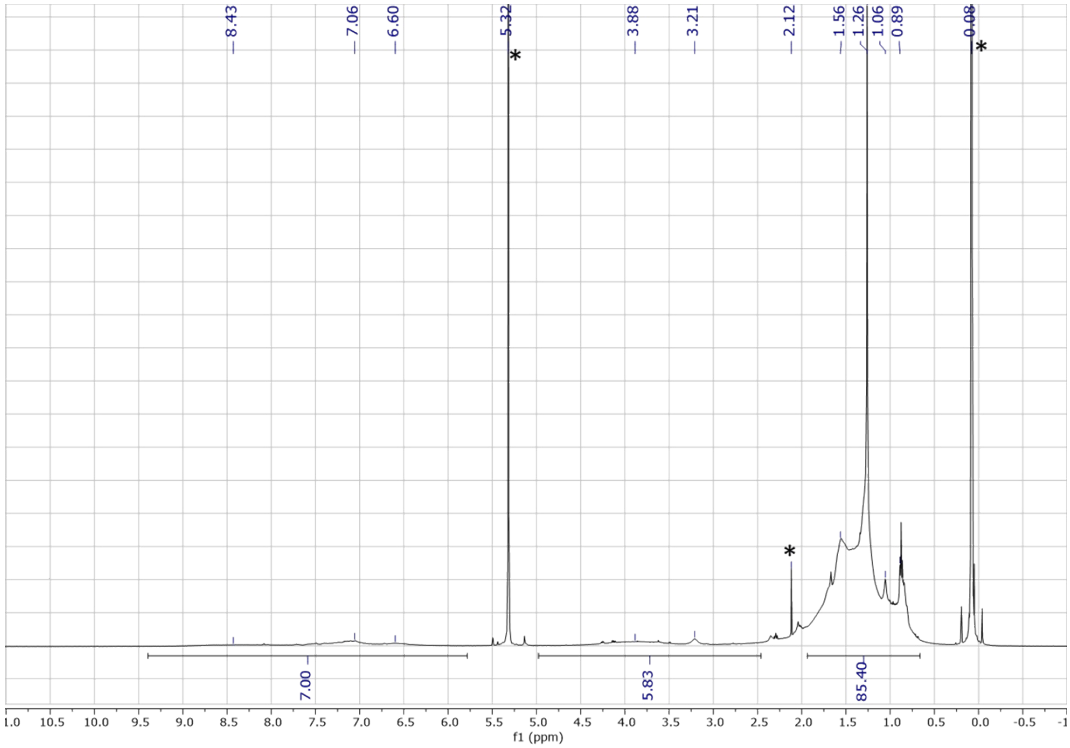
NMR Spectra of Polymer **P3**:



NMR Spectra of Polymer **P4**:

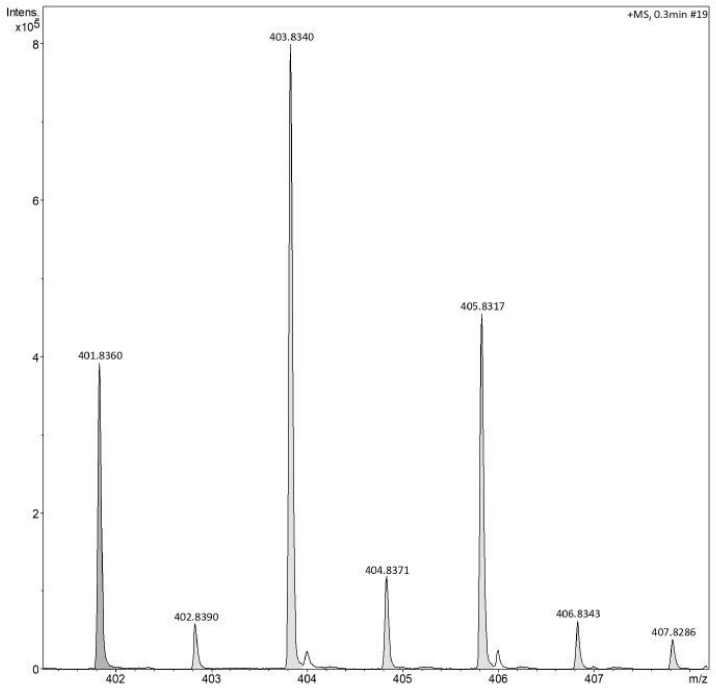


NMR Spectra of Polymer **P5**:



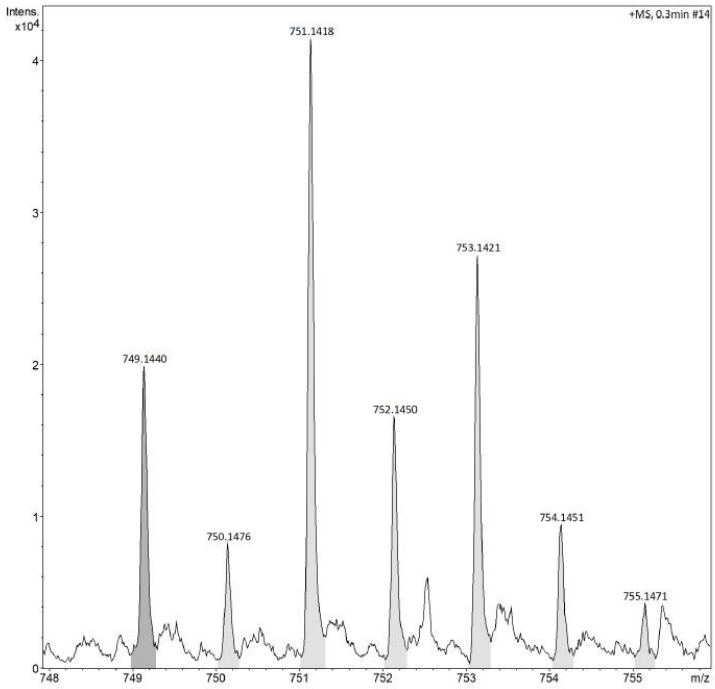
HR-ESI-MS of Compound **7**:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	rdb	N-Rule
401.8360	1	C11H6Br2N3S2	401.8364	1.0	9.5	ok



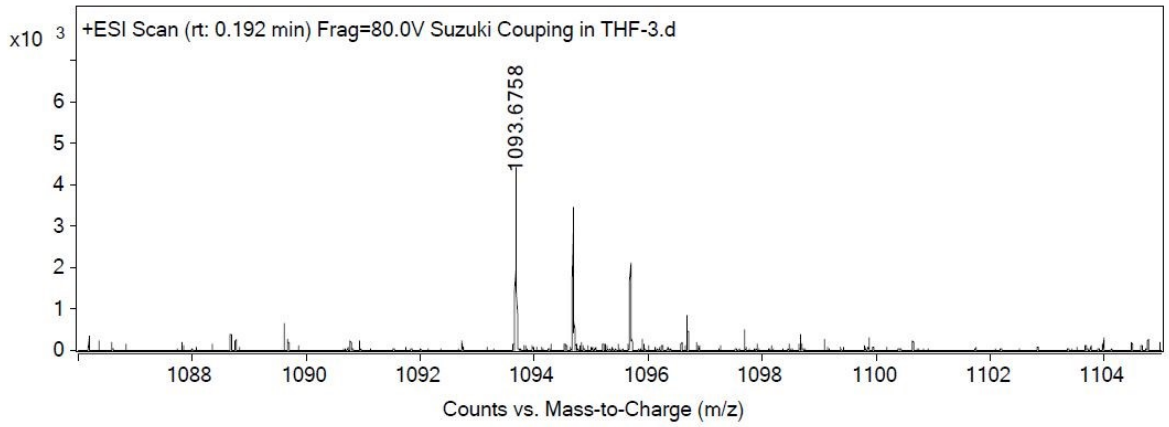
HR-ESI-MS of Compound **8**:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	rdb	N-Rule
749.1440	1	C35H47Br2N2O2S2	749.1440	0.1	12.5	ok



HR-ESI-MS of Compound **9**:

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
1093.6758	1	C67 H101 N2 O2 S4	1093.674	1.65



HR-ESI-MS of Compound **10**:

Meas. m/z	#	Formula	Calc. Mass	Err [ppm]
1249.4938	1	C67 H99 Br2 N2 O2 S4	1249.4950	-0.96