



Appendix

**Internal Coordinates of Poly(2-methylbut-2-enyl thiophene-3-carboxylate)
(PMT)**

Internal Coordinates	Internal Coordinates number	Internal Coordinates	Internal Coordinates number
$\nu[\text{C}\alpha=\text{C}\beta]$	1	$\phi[\text{C}\delta-\text{C}\varepsilon-\text{C}\xi]$	34
$\nu[\text{C}\alpha-\text{H}]$	2	$\phi[\text{C}\psi-\text{C}\varepsilon-\text{C}\xi]$	35
$\nu[\text{C}\beta-\text{C}\gamma]$	3	$\phi[\text{C}\varepsilon-\text{C}\psi-\text{S}]$	36
$\nu[\text{C}\beta-\text{C}\alpha]$	4	$\phi[\text{C}\varepsilon-\text{C}\psi-\text{H}]$	37
$\nu[\text{C}\gamma-\text{O}]$	5	$\phi[\text{S}-\text{C}\psi-\text{H}]$	38,41
$\nu[\text{C}\gamma-\text{H}]$	6,7	$\phi[\text{C}\psi-\text{S}-\text{C}\psi]$	39
$\nu[\text{O}-\text{C}\delta]$	8	$\phi[\text{S}-\text{C}\psi-\text{C}\xi]$	40
$\nu[\text{C}\delta-\text{C}\varepsilon]$	9	$\phi[\text{C}\xi-\text{C}\psi-\text{H}]$	42
$\nu[\text{C}\delta=\text{O}\delta]$	10	$\phi[\text{C}\varepsilon-\text{C}\xi-\text{C}\psi]$	43
$\nu[\text{C}\varepsilon=\text{C}\psi]$	11	$\phi[\text{C}\varepsilon-\text{C}\xi-\text{H}]$	44
$\nu[\text{C}\varepsilon-\text{C}\xi]$	12	$\phi[\text{C}\psi-\text{C}\xi-\text{H}]$	45
$\nu[\text{C}\psi-\text{S}]$	13,15	$\phi[\text{C}\beta-\text{C}\alpha=\text{C}\beta]$	46
$\nu[\text{C}\psi-\text{H}]$	14,17	$\phi[\text{C}\beta-\text{C}\alpha-\text{H}]$	47
$\nu[\text{C}\psi=\text{C}\xi]$	16	$\omega[\text{O}\delta=\text{C}\delta]$	48
$\nu[\text{C}\xi-\text{H}]$	18	$\omega[\text{H}-\text{C}\psi]$	49,50
$\phi[\text{C}\beta=\text{C}\alpha-\text{H}]$	19	$\omega[\text{H}-\text{C}\xi]$	51
$\phi[\text{C}\alpha=\text{C}\beta-\text{C}\gamma]$	20	$\omega[\text{H}-\text{C}\alpha]$	52
$\phi[\text{C}\alpha=\text{C}\beta-\text{C}\alpha]$	21	$\tau[\text{C}\beta-\text{C}\gamma]$	53
$\phi[\text{C}\gamma-\text{C}\beta-\text{C}\alpha]$	22	$\tau[\text{C}\gamma-\text{O}]$	54
$\phi[\text{C}\beta-\text{C}\gamma-\text{O}]$	23	$\tau[\text{O}-\text{C}\delta]$	55
$\phi[\text{C}\beta-\text{C}\gamma-\text{H}]$	24,25	$\tau[\text{C}\delta-\text{C}\varepsilon]$	56
$\phi[\text{O}-\text{C}\gamma-\text{H}]$	26,27	$\tau[\text{C}\varepsilon-\text{C}\psi]$	57
$\phi[\text{H}-\text{C}\gamma-\text{H}]$	28	$\tau[\text{C}\psi-\text{S}]$	58,59
$\phi[\text{C}\gamma-\text{O}-\text{C}\delta]$	29	$\tau[\text{C}\psi-\text{C}\xi]$	60
$\phi[\text{O}-\text{C}\delta-\text{C}\varepsilon]$	30	$\tau[\text{C}\xi-\text{C}\varepsilon]$	61
$\phi[\text{O}-\text{C}\delta=\text{O}\delta]$	31	$\tau[\text{C}\beta-\text{C}\alpha]$	62
$\phi[\text{C}\varepsilon-\text{C}\delta=\text{O}\delta]$	32	$\tau[\text{C}\alpha=\text{C}\beta]$	63
$\phi[\text{C}\delta-\text{C}\varepsilon-\text{C}\psi]$	33		

Note: ν , ϕ , ω and τ denote stretch, angle band, wag and torsion respectively. * and \$ corresponds to benzoid and quinoid rings respectively.

G and F Matrix Elements of Poly(2-methylbut-2-enyl thiophene-3-carboxylate) (PMT)

G_A

I	J	G(I,J)	I	J	G(I,J)	I	J	G(I,J)	I	J	G(I,J)
1	1	0.16651403	1	2	-0.03806566	1	3	-0.03973448	1	4	-0.04449172
1	19	-0.06789241	1	20	-0.04803215	1	21	-0.04809656	1	22	0.09576727
1	23	-0.03470023	1	24	0.04573355	1	25	-0.00905512	1	46	-0.03916882
1	47	0.03821881	1	52	0.03254127	1	53	-0.01189786	1	54	0.03527804
1	62	-0.02366527	1	63	0.03659408	2	1	-0.03806566	2	2	1.07532051
2	19	-0.05483999	2	20	0.05483729	2	21	-0.05467292	2	53	0.00061904
2	62	0.00506059	3	1	-0.03973448	3	3	0.16651403	3	4	-0.04036761
3	5	-0.02807922	3	6	-0.02971828	3	7	-0.02717191	3	19	0.05418411
3	20	-0.05418678	3	21	0.10354973	3	22	-0.04976702	3	23	-0.05476386
3	24	-0.07089752	3	25	-0.07180368	3	26	0.06319718	3	27	0.06592648
3	28	0.07125681	3	29	-0.05052875	3	46	0.03782058	3	47	-0.03672379
3	52	-0.03771233	3	54	-0.00948856	3	55	0.02315077	3	62	0.01901341
3	63	-0.04240917	4	1	-0.04449172	4	3	-0.04036761	4	4	0.16651403
4	19	-0.05196052	4	20	0.09954897	4	21	-0.05211930	4	22	-0.04780407
4	23	0.03721801	4	24	-0.04411094	4	25	0.00499219	4	46	-0.04703273
4	47	-0.07054034	4	52	0.00089731	4	53	0.01816512	4	54	-0.03186790
4	63	-0.00062942	5	3	-0.02807922	5	5	0.14578046	5	6	-0.02486674
5	7	-0.03105385	5	8	-0.02562582	5	20	-0.03717390	5	22	0.04006140
5	23	-0.05145621	5	24	0.06058466	5	25	0.06481847	5	26	-0.07243293
5	27	-0.07048127	5	28	0.07003986	5	29	-0.04188997	5	30	-0.04141558
5	31	0.04156183	5	48	-0.00567290	5	53	-0.01932247	5	55	0.00256673
5	56	-0.00679024	6	3	-0.02971828	6	5	-0.02486674	6	6	1.07532051
6	7	-0.02556337	6	20	0.04861453	6	22	-0.04711342	6	23	0.05261154
6	24	-0.05105792	6	25	0.06122916	6	26	-0.05551680	6	27	0.06006387
6	28	-0.07229373	6	29	0.00767242	6	53	0.05835235	6	54	-0.04009017
6	55	-0.06027973	7	3	-0.02717191	7	5	-0.03105385	7	6	-0.02556337
7	7	1.07532051	7	20	-0.00974013	7	22	0.00539547	7	23	0.05598611
7	24	0.06020386	7	25	-0.05166573	7	26	0.06246173	7	27	-0.05397415
7	28	-0.07223112	7	29	0.04358602	7	53	-0.03704240	7	54	0.04833038
7	55	0.03490111	8	5	-0.02562582	8	8	0.14578046	8	9	-0.03147135
8	10	-0.04709021	8	23	-0.03676603	8	26	0.00550694	8	27	0.03217834
8	29	-0.03984760	8	30	-0.05278313	8	31	-0.05602548	8	32	0.10876986
8	33	-0.05277899	8	34	0.05278224	8	48	0.00080464	8	53	0.01632149
8	54	-0.00550458	8	56	-0.00042250	8	57	0.00078408	8	61	0.00038336
9	8	-0.03147135	9	9	0.16651403	9	10	-0.04574537	9	11	-0.04486257
9	12	-0.05008836	9	29	-0.05597516	9	30	-0.05661632	9	31	0.11333812
9	32	-0.05676250	9	33	-0.05068264	9	34	-0.04628813	9	35	0.09695832
9	36	-0.05066390	9	37	0.05067621	9	43	-0.04627409	9	44	0.04628407
9	48	0.00078166	9	49	-0.00129847	9	51	0.00103899	9	54	-0.00931474
9	55	0.00381773	9	57	0.00058447	9	58	-0.00149683	9	60	0.00123764

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G_B

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F_A

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3	4	0.38401525	3	5	0.31555730	3	6	0.20910033	3	7	0.20465975
3	20	0.29353128	3	22	0.29745663	3	23	0.28836500	3	24	0.17837321
3	25	0.18134134	4	1	0.39496896	4	3	0.38401525	4	4	4.83382115
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8	8	6.20199804	8	9	0.35974592	8	10	0.64294266	8	29	0.25291094
8	30	0.28529484	8	31	0.39366216	9	8	0.35974592	9	9	4.70464683
9	10	0.46099124	9	11	0.43573289	9	12	0.24621211	9	30	0.30121334
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 25 25 0.69256462 26 5 0.14681091 26 6 0.11578109 26 26 0.66908485
 27 5 0.14120451 27 7 0.11439638 27 27 0.65642864 28 6 0.08220894
 28 7 0.08214698 28 28 0.49165038 29 5 0.26236338 29 8 0.25291094
 29 29 0.84028635 30 8 0.28529484 30 9 0.30121334 30 30 0.70703756
 31 8 0.39366216 31 10 0.37105863 31 31 0.87827605 32 9 0.30402847
 32 10 0.27463249 32 32 0.58171862 33 9 0.30084370 33 11 0.29146523
 33 33 0.64152874 34 9 0.15685730 34 12 0.15552077 34 34 0.39577349
 35 11 0.32195530 35 12 0.33192778 35 35 0.66968488 36 11 0.20221604
 36 13 0.23761749 36 36 0.50551190 37 11 0.19325430 37 14 0.16976555
 37 37 0.37744157 38 13 0.24149255 38 14 0.17928815 38 38 0.44933348
 39 13 0.30759465 39 15 0.30740259 39 39 0.89588479 40 15 0.23962143
 40 16 0.20212220 40 40 0.51010949 41 15 0.23999301 41 17 0.17877432
 41 41 0.44692416 42 16 0.19064255 42 17 0.16825283 42 42 0.37392111
 43 12 0.32560070 43 16 0.31517686 43 43 0.64736239 44 12 0.20645822
 44 18 0.17573536 44 44 0.41553861 45 16 0.20424201 45 18 0.17744867
 45 45 0.41357352 46 4 0.24552333 46 46 0.51544444 47 4 0.14234722
 47 47 0.42665449 48 48 0.34300000 49 49 0.25300000 50 50 0.25300000
 51 51 0.38500000 52 52 0.31050000 53 53 0.02500000 54 54 0.03000000
 55 55 0.03200000 56 56 0.01500000 57 57 0.05800000 58 58 0.02000000
 59 59 0.02000000 60 60 0.05800000 61 61 0.02800000 62 62 0.01800000
 63 63 0.01100000

F_B

4 1 0.42031666 4 2 0.17791611 46 1 0.23614415 47 2 0.11323575

- Note:**
1. Only nonzero elements are given. Also the elements of G_C , G_D and F_C , F_D are all zero.
 2. In order to economize the space, only G and F matrices are given only for PMT. Matrices for PMP can be provided on demand.