Supporting Information

Variation in charge transport properties, nonlinear and electro-optics of RM734 due to halogenation: A quantum mechanical study

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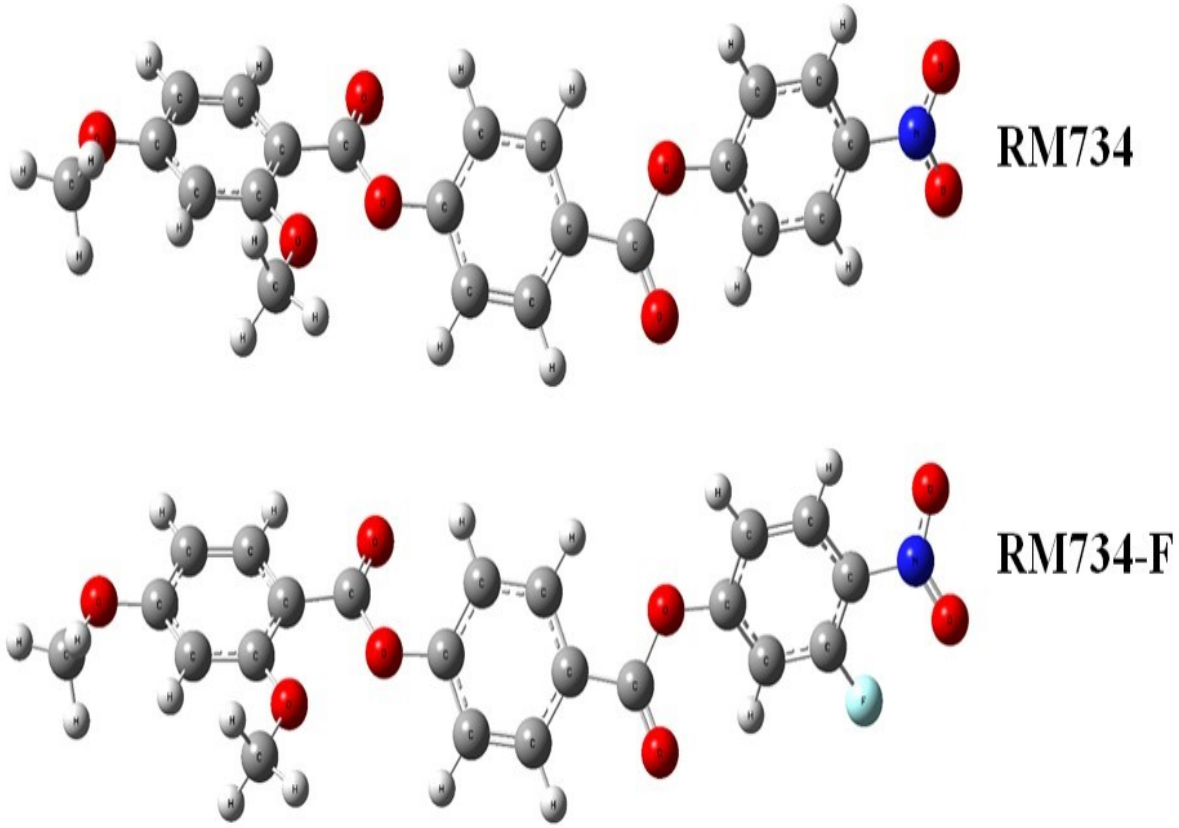
This supplement contains 23 pages, with 2 figures and 11 tables.

1. Optimized structure of RM734 and its halogen derivatives with labels



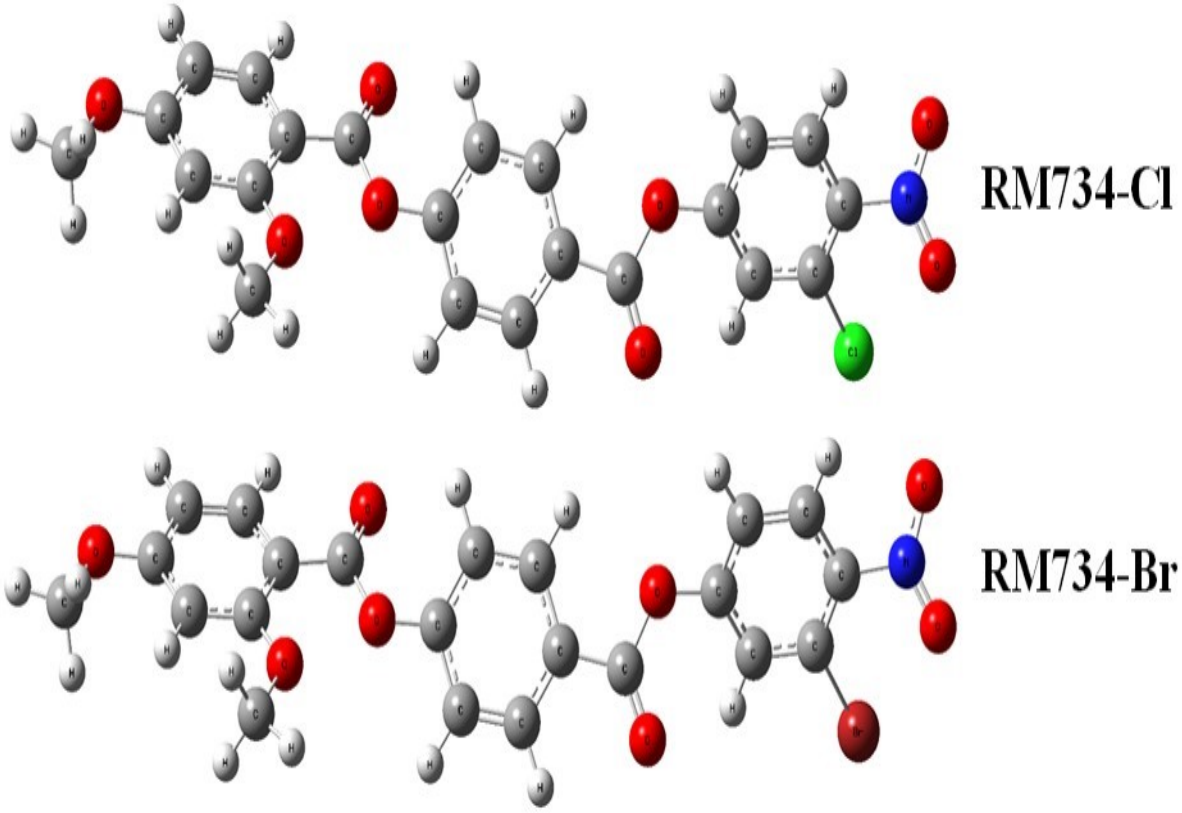


Figure S1. Optimized and labeled structure of RM734 liquid crystal molecule and its halogen derivatives.

2. Bond alteration

Table S1: - Bond length alteration for RM734.

Atoms	Bond length (Å)
C1-C2	1.4028
C1-C6	1.3971
C1-H7	1.0777
C2-C3	1.4172
C2-O15	1.3509
C3-C4	1.4078
C3-C20	1.4807
C4-C5	1.3779

C4-H8	1.0825
C5-C6	1.4011
C5-H9	1.0820
C6-O10	1.3535
O10-C11	1.4238
C11-H12	1.0891
C11-H13	1.0964
C11-H14	1.0965
O15-C16	1.4222
C16-H17	1.0965
C16-H18	1.0965
C16-H19	1.0891
C20-O21	1.2065
C20-O22	1.3728
O22-C23	1.3783
C23-C24	1.3971
C23-C25	1.3968
C24-C26	1.3891
C24-H27	1.0788
C25-C28	1.3851
C25-H29	1.0827
C26-C30	1.4009
C26-H31	1.0815
C28-C30	1.4017
C28-H32	1.0828
C30-C33	1.4793
C33-O34	1.2026
C33-O35	1.3816
O35-C36	1.3807
C36-C37	1.3960
C36-C38	1.3971
C37-C39	1.3872

C37-H40	1.0826
C38-C41	1.3892
C38-H42	1.0788
C39-C43	1.3922
C39-H44	1.0808
C41-C43	1.3918
C41-H45	1.0809
C43-N46	1.4764
N46-O47	1.2243
N46-O48	1.2246

Table S2: - Bond length alteration for **RM734-F**.

Atoms	Bond length (Å)
C1-C2	1.4028
C1-C6	1.3971
C1-H7	1.0777
C2-C3	1.4172
C2-O15	1.3509
C3-C4	1.4079
C3-C20	1.4802
C4-C5	1.3778
C4-H8	1.0825
C5-C6	1.4012
C5-H9	1.0820
C6-O10	1.3533
O10-C11	1.4239
C11-H12	1.0890
C11-H13	1.0964
C11-H14	1.0964
O15-C16	1.4224
C16-H17	1.0965
C16-H18	1.0965

C16-H19	1.0891
C20-O21	1.2064
C20-O22	1.3736
O22-C23	1.3774
C23-C24	1.3973
C23-C25	1.3971
C24-C26	1.3890
C24-H27	1.0788
C25-C28	1.3848
C25-H29	1.0827
C26-C30	1.4011
C26-H31	1.0814
C28-C30	1.4020
C28-H32	1.0827
C30-C33	1.4779
C33-O34	1.2021
C33-O35	1.3847
O35-C36	1.3761
C36-C37	1.3978
C36-C38	1.3933
C37-C39	1.3833
C37-H40	1.0819
C38-C41	1.3875
C38-H42	1.0783
C39-C43	1.3955
C39-H44	1.0811
C41-C43	1.3989
C41-F48	1.3337
C43-N45	1.4717
N45-O46	1.2208
N45-O47	1.226

Table S3: - Bond length alteration for **RM734-Cl**.

Atoms	Bond length (Å)
C1-C2	1.4028
C1-C6	1.3971
C1-H7	1.0777
C2-C3	1.4172
C2-O15	1.3509
C3-C4	1.4079
C3-C20	1.4803
C4-C5	1.3778
C4-H8	1.0825
C5-C6	1.4012
C5-H9	1.0820
C6-O10	1.3533
O10-C11	1.4239
C11-H12	1.0891
C11-H13	1.0964
C11-H14	1.0964
O15-C16	1.4223
C16-H17	1.0965
C16-H18	1.0965
C16-H19	1.0891
C20-O21	1.2064
C20-O22	1.3735
O22-C23	1.3775
C23-C24	1.3973
C23-C25	1.3971
C24-C26	1.3890
C24-H27	1.0787
C25-C28	1.3849
C25-H29	1.0827
C26-C30	1.4011

C26-H31	1.0814
C28-C30	1.402
C28-H32	1.0828
C30-C33	1.4780
C33-O34	1.2021
C33-O35	1.3845
O35-C36	1.3779
C36-C37	1.3948
C36-C38	1.3935
C37-C39	1.3837
C37-H40	1.0820
C38-C41	1.3932
C38-H42	1.0781
C39-C43	1.3941
C39-H44	1.0814
C41-C43	1.4005
C41-Cl48	1.7438
C43-N45	1.4768
N45-O46	1.2194
N45-O47	1.2251

Table S4: - Bond length alteration for **RM734-Br**.

Atoms	Bond length (Å)
C1-C2	1.4028
C1-C6	1.3971
C1-H7	1.0777
C2-C3	1.4173
C2-O15	1.3509
C3-C4	1.4079
C3-C20	1.4805
C4-C5	1.3778
C4-H8	1.0825

C5-C6	1.4012
C5-H9	1.0820
C6-O10	1.3533
O10-C11	1.4239
C11-H12	1.0891
C11-H13	1.0964
C11-H14	1.0965
O15-C16	1.4223
C16-H17	1.0964
C16-H18	1.0965
C16-H19	1.0891
C20-O21	1.2065
C20-O22	1.3730
O22-C23	1.3775
C23-C24	1.3975
C23-C25	1.3973
C24-C26	1.3892
C24-H27	1.0786
C25-C28	1.3847
C25-H29	1.0827
C26-C30	1.4009
C26-H31	1.0814
C28-C30	1.4020
C28-H32	1.0828
C30-C33	1.4780
C33-O34	1.2021
C33-O35	1.3847
O35-C36	1.3785
C36-C37	1.3940
C36-C38	1.3938
C37-C39	1.3840
C37-H40	1.0821

C38-C41	1.3936
C38-H42	1.0781
C39-C43	1.3945
C39-H44	1.0815
C41-C43	1.4001
C41-Br48	1.9068
C43-N45	1.4778
N45-O46	1.2194
N45-O47	1.2250

Table S5: - Bond angle alteration for **RM734.**

Atoms	Angle (in Degrees)
A(2,1,6)	120.5397
A(2,1,7)	119.6515
A(6,1,7)	119.8084
A(1,2,3)	119.7777
A(1,2,15)	121.6226
A(3,2,15)	118.5958
A(2,3,4)	117.7908
A(2,3,20)	127.0539
A(4,3,20)	115.1528
A(3,4,5)	122.7608
A(3,4,8)	117.1526
A(5,4,8)	120.0865
A(4,5,6)	118.8783
A(4,5,9)	121.9658
A(6,5,9)	119.1560
A(1,6,5)	120.2495
A(1,6,10)	123.7720
A(5,6,10)	115.9784
A(6,10,11)	118.5833
A(10,11,12)	105.8440

A(10,11,13)	111.0127
A(10,11,14)	111.0127
A(12,11,13)	109.7320
A(12,11,14)	109.7236
A(13,11,14)	109.4553
A(2,15,16)	119.1963
A(15,16,17)	111.1840
A(15,16,18)	111.1973
A(15,16,19)	105.5069
A(17,16,18)	109.4770
A(17,16,19)	109.6960
A(18,16,19)	109.7057
A(3,20,21)	124.1937
A(3,20,22)	112.9179
A(21,20,22)	122.8691
A(20,22,23)	122.7557
A(22,23,24)	124.1720
A(22,23,25)	114.8311
A(24,23,25)	120.8738
A(23,24,26)	118.9740
A(23,24,27)	120.3047
A(26,24,27)	120.7131
A(23,25,28)	119.7220
A(23,25,29)	118.6584
A(28,25,29)	121.6195
A(24,26,30)	120.8014
A(24,26,31)	119.5676
A(30,26,31)	119.6309
A(25,28,30)	120.2301
A(25,28,32)	120.9236
A(30,28,32)	118.8462
A(26,30,28)	119.3979

A(26,30,33)	123.0934
A(28,30,33)	117.5088
A(30,33,34)	125.5473
A(30,33,35)	111.0639
A(34,33,35)	123.3869
A(33,35,36)	122.4235
A(35,36,37)	115.2204
A(35,36,38)	123.5524
A(37,36,38)	121.1212
A(36,37,39)	119.8503
A(36,37,40)	119.0046
A(39,37,40)	121.1450
A(36,38,41)	119.0065
A(36,38,42)	120.4328
A(41,38,42)	120.5549
A(37,39,43)	118.7692
A(37,39,44)	121.6532
A(43,39,44)	119.5774
A(38,41,43)	119.5062
A(38,41,45)	121.1335
A(43,41,45)	119.3602
A(39,43,41)	121.7461
A(39,43,46)	119.0913
A(41,43,46)	119.1624
A(43,46,47)	117.6901
A(43,46,48)	117.6387
A(47,46,48)	124.6712

Table S6: - Bond angle alteration for **RM734-F.**

Atoms	Angle (in Degrees)
A(2,1,6)	120.5407
A(2,1,7)	119.6534

A(6,1,7)	119.8055
A(1,2,3)	119.7724
A(1,2,15)	121.6252
A(3,2,15)	118.5982
A(2,3,4)	117.7978
A(2,3,20)	127.0525
A(4,3,20)	115.1471
A(3,4,5)	122.7539
A(3,4,8)	117.1608
A(5,4,8)	120.0852
A(4,5,6)	118.8799
A(4,5,9)	121.9663
A(6,5,9)	119.1538
A(1,6,5)	120.2517
A(1,6,10)	123.7747
A(5,6,10)	115.9734
A(6,10,11)	118.5984
A(10,11,12)	105.8397
A(10,11,13)	111.0098
A(10,11,14)	111.0055
A(12,11,13)	109.7325
A(12,11,14)	109.7261
A(13,11,14)	109.4663
A(2,15,16)	119.1928
A(15,16,17)	111.1759
A(15,16,18)	111.1917
A(15,16,19)	105.5081
A(17,16,18)	109.4845
A(17,16,19)	109.7009
A(18,16,19)	109.7059
A(3,20,21)	124.2482
A(3,20,22)	112.9056

A(21,20,22)	122.8258
A(20,22,23)	122.8050
A(22,23,24)	124.2185
A(22,23,25)	114.8057
A(24,23,25)	120.8548
A(23,24,26)	118.9856
A(23,24,27)	120.3027
A(26,24,27)	120.7035
A(23,25,28)	119.740
A(23,25,29)	118.6533
A(28,25,29)	121.6066
A(24,26,30)	120.7984
A(24,26,31)	119.5235
A(30,26,31)	119.6780
A(25,28,30)	120.2231
A(25,28,32)	120.8969
A(30,28,32)	118.8800
A(26,30,28)	119.3973
A(26,30,33)	123.1626
A(28,30,33)	117.4402
A(30,33,34)	125.6842
A(30,33,35)	110.9833
A(34,33,35)	123.3307
A(33,35,36)	123.1423
A(35,36,37)	115.1009
A(35,36,38)	123.8756
A(37,36,38)	120.9140
A(36,37,39)	119.4734
A(36,37,40)	119.2553
A(39,37,40)	121.2713
A(36,38,41)	118.8984
A(36,38,42)	122.1632

A(41,38,42)	118.9336
A(37,39,43)	120.5165
A(37,39,44)	121.3916
A(43,39,44)	118.0919
A(38,41,43)	120.9182
A(38,41,45)	117.2788
A(43,41,45)	121.7801
A(39,43,41)	119.2678
A(39,43,46)	118.2730
A(41,43,46)	122.4580
A(43,46,47)	118.0119
A(43,46,48)	116.8982
A(47,46,48)	125.0829

Table S7: - Bond angle alteration for **RM734-Cl.**

Atoms	Angle (in Degrees)
A(2,1,6)	120.5414
A(2,1,7)	119.6520
A(6,1,7)	119.8063
A(1,2,3)	119.7734
A(1,2,15)	121.6205
A(3,2,15)	118.6021
A(2,3,4)	117.7937
A(2,3,20)	127.0624
A(4,3,20)	115.1412
A(3,4,5)	122.7578
A(3,4,8)	117.1590
A(5,4,8)	120.0831
A(4,5,6)	118.8797
A(4,5,9)	121.9667
A(6,5,9)	119.1536

A(1,6,5)	120.2508
A(1,6,10)	123.7761
A(5,6,10)	115.9729
A(6,10,11)	118.5972
A(10,11,12)	105.8422
A(10,11,13)	111.0108
A(10,11,14)	111.0087
A(12,11,13)	109.7320
A(12,11,14)	109.7244
A(13,11,14)	109.4619
A(2,15,16)	119.1958
A(15,16,17)	111.1784
A(15,16,18)	111.1931
A(15,16,19)	105.5097
A(17,16,18)	109.4811
A(17,16,19)	109.6989
A(18,16,19)	109.7058
A(3,20,21)	124.2324
A(3,20,22)	112.9122
A(21,20,22)	122.8363
A(20,22,23)	122.8241
A(22,23,24)	124.2235
A(22,23,25)	114.7949
A(24,23,25)	120.8593
A(23,24,26)	118.9780
A(23,24,27)	120.3126
A(26,24,27)	120.7013
A(23,25,28)	119.7404
A(23,25,29)	118.6502
A(28,25,29)	121.6092
A(24,26,30)	120.8012
A(24,26,31)	119.5316

A(30,26,31)	119.6671
A(25,28,30)	120.2150
A(25,28,32)	120.9093
A(30,28,32)	118.8757
A(26,30,28)	119.4054
A(26,30,33)	123.1258
A(28,30,33)	117.4688
A(30,33,34)	125.7236
A(30,33,35)	111.0210
A(34,33,35)	123.2539
A(33,35,36)	122.6514
A(35,36,37)	115.4319
A(35,36,38)	123.4650
A(37,36,38)	120.9719
A(36,37,39)	119.2156
A(36,37,40)	119.4512
A(39,37,40)	121.3326
A(36,38,41)	119.6080
A(36,38,42)	120.7519
A(41,38,42)	119.6378
A(37,39,43)	120.4998
A(37,39,44)	121.2150
A(43,39,44)	118.2851
A(38,41,43)	119.5392
A(38,41,48)	117.0690
A(43,41,48)	123.3173
A(39,43,41)	120.1346
A(39,43,45)	116.3947
A(41,43,45)	123.4682
A(43,45,46)	118.0441
A(43,45,47)	116.5933
A(46,45,47)	125.3365

Table S8: - Bond angle alteration for **RM734-Br.**

Atoms	Angle (in Degree)
A(2,1,6)	120.5469
A(2,1,7)	119.6418
A(6,1,7)	119.8109
A(1,2,3)	119.7745
A(1,2,15)	121.6153
A(3,2,15)	118.6067
A(2,3,4)	117.7865
A(2,3,20)	127.0645
A(4,3,20)	115.1471
A(3,4,5)	122.7630
A(3,4,8)	117.1608
A(5,4,8)	120.0761
A(4,5,6)	118.8811
A(4,5,9)	121.9644
A(6,5,9)	119.1545
A(1,6,5)	120.2449
A(1,6,10)	123.7733
A(5,6,10)	115.9816
A(6,10,11)	118.5838
A(10,11,12)	105.8422
A(10,11,13)	111.0001
A(10,11,14)	111.0176
A(12,11,13)	109.7401
A(12,11,14)	109.7220
A(13,11,14)	109.4582
A(2,15,16)	119.2022
A(15,16,17)	111.1934
A(15,16,18)	111.1946
A(15,16,19)	105.5066
A(17,16,18)	109.4830

A(17,16,19)	109.6845
A(18,16,19)	109.7043
A(3,20,21)	124.2097
A(3,20,22)	112.8766
A(21,20,22)	122.8954
A(20,22,23)	123.0493
A(22,23,24)	124.3819
A(22,23,25)	114.6430
A(24,23,25)	120.8554
A(23,24,26)	118.9492
A(23,24,27)	120.3458
A(26,24,27)	120.6971
A(23,25,28)	119.7588
A(23,25,29)	118.6185
A(28,25,29)	121.6226
A(24,26,30)	120.8243
A(24,26,31)	119.5398
A(30,26,31)	119.6358
A(25,28,30)	120.1976
A(25,28,32)	120.9336
A(30,28,32)	118.8687
A(26,30,28)	119.4138
A(26,30,33)	123.1042
A(28,30,33)	117.4820
A(30,33,34)	125.7341
A(30,33,35)	111.0585
A(34,33,35)	123.2060
A(33,35,36)	122.3175
A(35,36,37)	115.6406
A(35,36,38)	123.1966
A(37,36,38)	121.0270
A(36,37,39)	119.1473

A(36,37,40)	119.5044
A(39,37,40)	121.3477
A(36,38,41)	119.6613
A(36,38,42)	120.3538
A(41,38,42)	119.9822
A(37,39,43)	120.4940
A(37,39,44)	121.1863
A(43,39,44)	118.3196
A(38,41,43)	119.3960
A(38,41,48)	116.5400
A(43,41,48)	123.9644
A(39,43,41)	120.2405
A(39,43,45)	116.0858
A(41,43,45)	123.6713
A(43,45,46)	118.0424
A(43,45,47)	116.6159
A(46,45,47)	120.5469

3. RESP Charges

Table S9: - RESP charges on individual atom for RM734, RM734-F. RM734-Cl and RM734-Br.

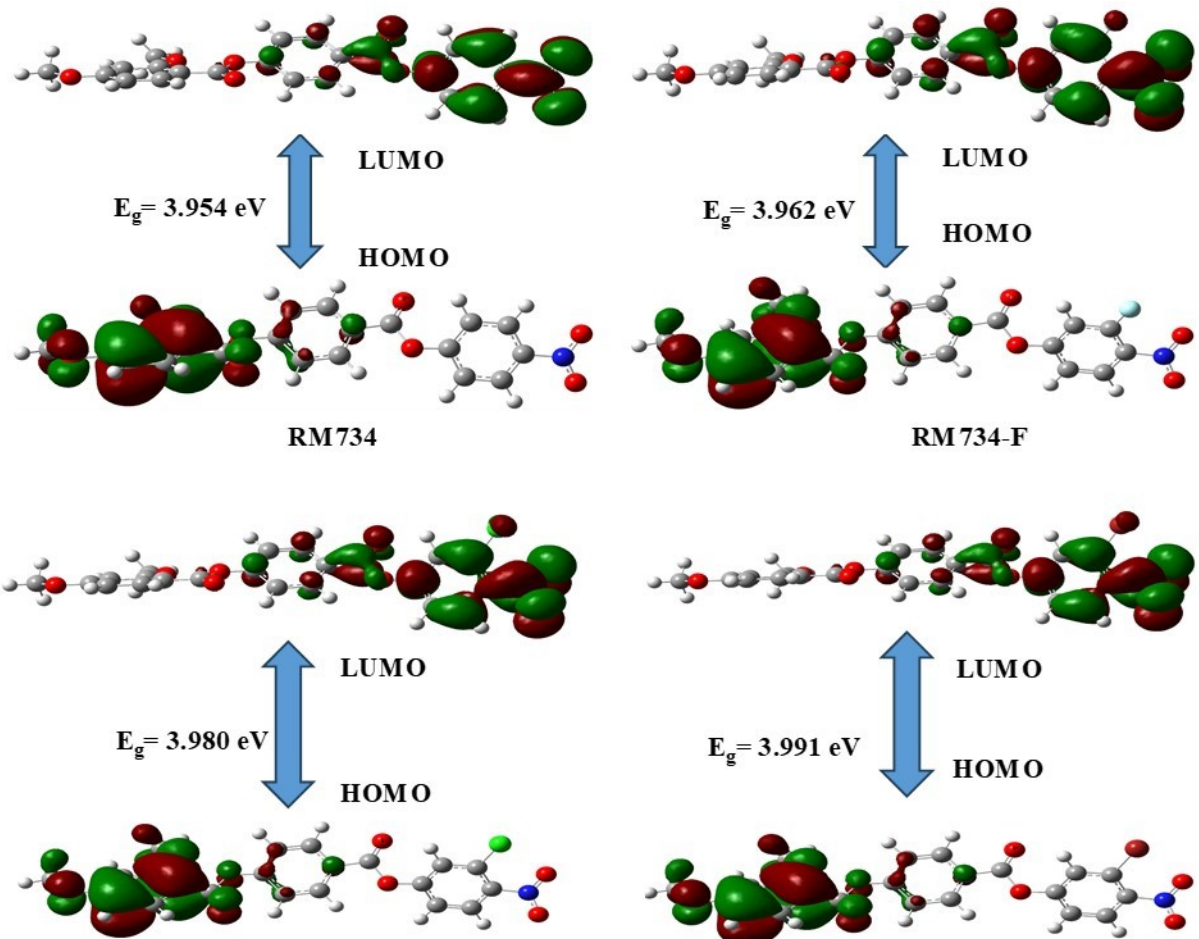
Atoms	RM734	RM734-F	RM734-Cl	RM734-Br
C01	-0.46987	-0.47226	-0.47185	-0.47651
C02	0.48081	0.48231	0.48368	0.48857
C03	-0.52709	-0.53354	-0.53705	-0.53277
C04	0.06424	0.06651	0.06723	0.06802
C05	-0.47354	-0.47456	-0.47459	-0.47861
C06	0.53581	0.53817	0.53777	0.54153
H07	0.19862	0.19939	0.19855	0.19974
H08	0.14814	0.14714	0.14712	0.14739
H09	0.20098	0.2017	0.20179	0.20265

O10	-0.37761	-0.37905	-0.37803	-0.37883
C11	-0.01256	-0.00658	-0.01049	-0.01263
H12	0.09255	0.09105	0.09221	0.0928
H13	0.09255	0.09105	0.09221	0.0928
H14	0.09255	0.09105	0.09221	0.0928
O15	-0.27153	-0.26751	-0.26693	-0.27292
C16	-0.16403	-0.17161	-0.17513	-0.16911
H17	0.12648	0.12822	0.12927	0.12802
H18	0.12648	0.12822	0.12927	0.12802
H19	0.12648	0.12822	0.12927	0.12802
C20	0.93292	0.93835	0.94295	0.9332
O21	-0.66531	-0.66392	-0.66522	-0.66289
O22	-0.52567	-0.52578	-0.52662	-0.52413
C23	0.45392	0.45089	0.44853	0.4517
C24	-0.28985	-0.28713	-0.28545	-0.28961
C25	-0.25681	-0.2538	-0.24938	-0.2521
C26	-0.07902	-0.07791	-0.08008	-0.07617
H27	0.20426	0.20568	0.20489	0.20478
C28	-0.10259	-0.09763	-0.10113	-0.10013
H29	0.19676	0.19474	0.1936	0.19576
C30	-0.17052	-0.17877	-0.18108	-0.18264
H31	0.16133	0.15764	0.16005	0.16104
H32	0.16057	0.15991	0.15982	0.1585
C33	0.80637	0.80514	0.82004	0.82365
O34	-0.60707	-0.60019	-0.60491	-0.60405
O35	-0.46593	-0.44376	-0.45138	-0.45932
C36	0.45483	0.49967	0.40426	0.40235
C37	-0.23453	-0.28021	-0.18203	-0.17919
C38	-0.2848	-0.45231	-0.20432	-0.15419
C39	-0.12374	-0.10878	-0.21555	-0.22956
H40	0.19558	0.20479	0.19335	0.19452
C41	-0.10328	0.39387	-0.00849	-0.11643

H42	0.22176	0.26875	0.20772	0.1841
C43	-0.07466	-0.21807	0.01207	0.07358
H44	0.18545	0.20796	0.22252	0.22541
H45/F45/Cl45/Br45	0.17958	-0.17437	-0.0634	-0.01508
N46	0.83553	0.89433	0.82172	0.78513
O47	-0.49684	-0.49713	-0.47025	-0.45178
O48	-0.49773	-0.50991	-0.48874	-0.48548

4. HOME AND LUMO

Figure S2. HOMO and LUMO diagram of RM734 and its halogen derivatives.



5. Nonlinear optical properties of urea and thiourea

For compression basis, the nonlinear optical properties of urea and thiourea has been also

Table S10:- Nonlinear optical properties of urea and thiourea using B3LYP/6-311G**.

calculated using B3LYP/6-311G** and B3LYP/def2-TZVPD methodologies.

Parameters	**Urea**	**Thiourea**
Anisotropy in Polarizability $(\Delta\alpha) \times 10^{-24}$ esu	2.499	6.486
First order Hyperpolarizability $(\beta_{total}) \times 10^{-33}$ esu	816.876	1669.474
Second order Hyperpolarizability $\langle\gamma\rangle \times 10^{-36}$ esu	1.249	2.896

Table S11:- Nonlinear optical properties of urea and thiourea using B3LYP/def2-TZVPD.

Parameters	**Urea**	**Thiourea**
Anisotropy in Polarizability $(\Delta\alpha) \times 10^{-24}$ esu	2.173	4.310
First order Hyperpolarizability $(\beta_{total}) \times 10^{-33}$ esu	673.459	554.318
Second order Hyperpolarizability $\langle\gamma\rangle \times 10^{-36}$ esu	3.833	11.237