

# Opening access to new chiral macrocycles: from allenes to spiranes

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DFT energies and number of imaginary frequencies

	CAM-B3LYP/6-31G*		M062x/6-31G*	
	SCF Energy	N. Imag.	SCF Energy	N. Imag.
(P <sub>4</sub> )-DEA	-1384.78609266	0	-1385.02539388	0
(P <sub>4</sub> )-DES	-4451.23457228	0	-4452.0543129	0
(P <sub>2</sub> )-DEAp	-939.32304450	0	-939.47749723	0
(P <sub>2</sub> )-DESp	-2472.55921778	0	-2473.00417990	0
(P <sub>2</sub> )-DEA <sub>bp</sub>	-1186.29582271	0	-1186.48602605	0
(P <sub>2</sub> )-DES <sub>bp</sub>	-2719.52272382	0	-2720.00368506	0
(P)-DEA	-347.36050390	0	-347.41673671	0
(P)-DES	-1113.97158027	0	-1114.17295098	0

CAM-B3LYP/6-31G\* XYZ geometries ( Å ):

(P<sub>4</sub>)-DEA

C	0.66924	-4.91441	0.14442
C	-0.66924	-4.91441	-0.14442
C	1.85373	-4.8717	0.39384
C	-1.85373	-4.8717	-0.39384
C	3.24169	-4.78615	0.72977
C	4.03121	-4.03121	0.
C	-3.24169	-4.78615	-0.72977
C	-4.03121	-4.03121	0.
C	4.78615	-3.24169	-0.72977
C	-4.78615	-3.24169	0.72977
C	4.8717	-1.85373	-0.39384
C	4.91441	-0.66924	-0.14442

C	-4.8717	-1.85373	0.39384
C	-4.91441	-0.66924	0.14442
C	4.91441	0.66924	0.14442
C	4.8717	1.85373	0.39384
C	4.78615	3.24169	0.72977
C	4.03121	4.03121	0.
C	3.24169	4.78615	-0.72977
C	1.85373	4.8717	-0.39384
C	0.66924	4.91441	-0.14442
C	-0.66924	4.91441	0.14442
C	-1.85373	4.8717	0.39384
C	-3.24169	4.78615	0.72977
C	-4.03121	4.03121	0.
C	-4.78615	3.24169	-0.72977
C	-4.8717	1.85373	-0.39384
C	-4.91441	0.66924	-0.14442
C	5.55714	3.72912	1.93786
H	5.2406	3.18441	2.83237
H	6.62867	3.55262	1.80314
H	5.39121	4.79609	2.09667
C	3.72912	5.55714	-1.93786
H	3.18441	5.2406	-2.83237
H	3.55262	6.62867	-1.80314
H	4.79609	5.39121	-2.09667
C	-5.55714	3.72912	-1.93786
H	-5.2406	3.18441	-2.83237
H	-6.62867	3.55262	-1.80314
H	-5.39121	4.79609	-2.09667
C	-3.72912	5.55714	1.93786
H	-3.18441	5.2406	2.83237
H	-3.55262	6.62867	1.80314
H	-4.79609	5.39121	2.09667
C	3.72912	-5.55714	1.93786
H	3.18441	-5.2406	2.83237
H	3.55262	-6.62867	1.80314
H	4.79609	-5.39121	2.09667
C	5.55714	-3.72912	-1.93786
H	5.2406	-3.18441	-2.83237
H	6.62867	-3.55262	-1.80314
H	5.39121	-4.79609	-2.09667
C	-3.72912	-5.55714	-1.93786
H	-3.18441	-5.2406	-2.83237
H	-3.55262	-6.62867	-1.80314
H	-4.79609	-5.39121	-2.09667
C	-5.55714	-3.72912	1.93786
H	-5.2406	-3.18441	2.83237
H	-6.62867	-3.55262	1.80314
H	-5.39121	-4.79609	2.09667

**(P<sub>4</sub>)-DES**

C	5.83696	2.36063	3.3961
C	5.82789	3.44991	4.26496
C	6.05024	4.72433	3.74699
C	6.28174	4.90166	2.36841

C	6.29257	3.8292	1.49767
C	6.06614	2.53745	2.01662
H	5.66454	1.35923	3.77005
H	5.64797	3.30333	5.32347
H	6.46874	3.96879	0.43759
C	6.50115	6.37994	2.05082
C	6.35217	7.02509	3.42706
C	6.44437	8.36583	3.76495
C	6.09373	6.04608	4.40552
C	6.27362	8.72899	5.10599
H	6.64231	9.11106	3.00286
C	5.92471	6.40733	5.73993
C	6.01706	7.75943	6.08165
H	6.33943	9.7716	5.39176
H	5.72521	5.65845	6.49775
H	5.88768	8.06163	7.11367
C	7.85302	6.65871	1.39664
C	9.11958	6.37594	1.88239
C	7.67719	7.282	0.14647
C	10.22694	6.72478	1.10029
H	9.2424	5.89494	2.84626
C	8.77901	7.6297	-0.63148
C	10.05693	7.34471	-0.14265
H	11.22626	6.51203	1.45993
H	8.65059	8.10931	-1.59511
H	10.92713	7.60601	-0.73272
C	5.52654	6.92692	1.00987
C	6.22907	7.44819	-0.0951
C	4.14583	6.94615	1.05683
C	5.53827	7.99802	-1.17306
C	3.44207	7.50191	-0.03167
H	3.60732	6.54288	1.90652
C	4.14554	8.0222	-1.13649
H	6.07	8.39999	-2.02757
C	2.01526	7.53628	-0.01947
H	3.58215	8.44276	-1.9599
C	6.06276	1.40554	1.14812
C	6.05335	0.44223	0.41013
C	0.80219	7.56185	-0.00807
C	4.14554	-8.0222	1.13649
C	5.53827	-7.99802	1.17306
C	6.22907	-7.44819	0.0951
C	5.52654	-6.92692	-1.00987
C	4.14583	-6.94615	-1.05683
C	3.44207	-7.50191	0.03167
H	3.58215	-8.44276	1.9599
H	6.07	-8.39999	2.02757
H	3.60732	-6.54288	-1.90652
C	6.50115	-6.37994	-2.05082
C	7.85302	-6.65871	-1.39664
C	9.11958	-6.37594	-1.88239
C	7.67719	-7.282	-0.14647
C	10.22694	-6.72478	-1.10029
H	9.2424	-5.89494	-2.84626
C	8.77901	-7.6297	0.63148
C	10.05693	-7.34471	0.14265

H	11.22626	-6.51203	-1.45993
H	8.65059	-8.10931	1.59511
H	10.92713	-7.60601	0.73272
C	6.35217	-7.02509	-3.42706
C	6.44437	-8.36583	-3.76495
C	6.09373	-6.04608	-4.40552
C	6.27362	-8.72899	-5.10599
H	6.64231	-9.11106	-3.00286
C	5.92471	-6.40733	-5.73993
C	6.01706	-7.75943	-6.08165
H	6.33943	-9.7716	-5.39176
H	5.72521	-5.65845	-6.49775
H	5.88768	-8.06163	-7.11367
C	6.28174	-4.90166	-2.36841
C	6.05024	-4.72433	-3.74699
C	6.29257	-3.8292	-1.49767
C	5.82789	-3.44991	-4.26496
C	6.06614	-2.53745	-2.01662
H	6.46874	-3.96879	-0.43759
C	5.83696	-2.36063	-3.3961
H	5.64797	-3.30333	-5.32347
C	6.06276	-1.40554	-1.14812
H	5.66454	-1.35923	-3.77005
C	2.01526	-7.53628	0.01947
C	0.80219	-7.56185	0.00807
C	6.05335	-0.44223	-0.41013
C	-5.83696	2.36063	-3.3961
C	-5.82789	3.44991	-4.26496
C	-6.05024	4.72433	-3.74699
C	-6.28174	4.90166	-2.36841
C	-6.29257	3.8292	-1.49767
C	-6.06614	2.53745	-2.01662
H	-5.66454	1.35923	-3.77005
H	-5.64797	3.30333	-5.32347
H	-6.46874	3.96879	-0.43759
C	-6.50115	6.37994	-2.05082
C	-6.35217	7.02509	-3.42706
C	-6.44437	8.36583	-3.76495
C	-6.09373	6.04608	-4.40552
C	-6.27362	8.72899	-5.10599
H	-6.64231	9.11106	-3.00286
C	-5.92471	6.40733	-5.73993
C	-6.01706	7.75943	-6.08165
H	-6.33943	9.7716	-5.39176
H	-5.72521	5.65845	-6.49775
H	-5.88768	8.06163	-7.11367
C	-7.85302	6.65871	-1.39664
C	-9.11958	6.37594	-1.88239
C	-7.67719	7.282	-0.14647
C	-10.22694	6.72478	-1.10029
H	-9.2424	5.89494	-2.84626
C	-8.77901	7.6297	0.63148
C	-10.05693	7.34471	0.14265
H	-11.22626	6.51203	-1.45993
H	-8.65059	8.10931	1.59511
H	-10.92713	7.60601	0.73272

C	-5.52654	6.92692	-1.00987
C	-6.22907	7.44819	0.0951
C	-4.14583	6.94615	-1.05683
C	-5.53827	7.99802	1.17306
C	-3.44207	7.50191	0.03167
H	-3.60732	6.54288	-1.90652
C	-4.14554	8.0222	1.13649
H	-6.07	8.39999	2.02757
C	-2.01526	7.53628	0.01947
H	-3.58215	8.44276	1.9599
C	-6.06276	1.40554	-1.14812
C	-6.05335	0.44223	-0.41013
C	-0.80219	7.56185	0.00807
C	-4.14554	-8.0222	-1.13649
C	-5.53827	-7.99802	-1.17306
C	-6.22907	-7.44819	-0.0951
C	-5.52654	-6.92692	1.00987
C	-4.14583	-6.94615	1.05683
C	-3.44207	-7.50191	-0.03167
H	-3.58215	-8.44276	-1.9599
H	-6.07	-8.39999	-2.02757
H	-3.60732	-6.54288	1.90652
C	-6.50115	-6.37994	2.05082
C	-7.85302	-6.65871	1.39664
C	-9.11958	-6.37594	1.88239
C	-7.67719	-7.282	0.14647
C	-10.22694	-6.72478	1.10029
H	-9.2424	-5.89494	2.84626
C	-8.77901	-7.6297	-0.63148
C	-10.05693	-7.34471	-0.14265
H	-11.22626	-6.51203	1.45993
H	-8.65059	-8.10931	-1.59511
H	-10.92713	-7.60601	-0.73272
C	-6.35217	-7.02509	3.42706
C	-6.44437	-8.36583	3.76495
C	-6.09373	-6.04608	4.40552
C	-6.27362	-8.72899	5.10599
H	-6.64231	-9.11106	3.00286
C	-5.92471	-6.40733	5.73993
C	-6.01706	-7.75943	6.08165
H	-6.33943	-9.7716	5.39176
H	-5.72521	-5.65845	6.49775
H	-5.88768	-8.06163	7.11367
C	-6.28174	-4.90166	2.36841
C	-6.05024	-4.72433	3.74699
C	-6.29257	-3.8292	1.49767
C	-5.82789	-3.44991	4.26496
C	-6.06614	-2.53745	2.01662
H	-6.46874	-3.96879	0.43759
C	-5.83696	-2.36063	3.3961
H	-5.64797	-3.30333	5.32347
C	-6.06276	-1.40554	1.14812
H	-5.66454	-1.35923	3.77005
C	-2.01526	-7.53628	-0.01947
C	-0.80219	-7.56185	-0.00807
C	-6.05335	-0.44223	0.41013

**(P<sub>2</sub>)-DEAp**

C	0.11745	-1.19391	4.04225
C	0.	0.	4.74063
H	0.20992	-2.14457	4.55469
C	-0.11465	1.14553	2.64516
C	-0.11745	1.19391	4.04225
H	0.	0.	5.82611
H	-0.20992	2.14457	4.55469
N	0.	0.	1.96534
C	-0.24611	2.31038	1.81195
C	-0.37226	3.11288	0.91685
C	-0.57783	3.89383	-0.2716
C	0.18711	3.58164	-1.2943
C	0.93828	3.08002	-2.25042
C	0.51607	1.80875	-2.7639
C	0.11465	-1.14553	2.64516
C	0.24611	-2.31038	1.81195
C	0.37226	-3.11288	0.91685
C	0.57783	-3.89383	-0.2716
C	-0.18711	-3.58164	-1.2943
C	-0.93828	-3.08002	-2.25042
C	-0.51607	-1.80875	-2.7639
C	-0.18722	-0.65893	-2.9676
C	0.18722	0.65893	-2.9676
C	-1.72471	4.92089	-0.30943
H	-2.50796	4.60526	0.34769
H	-1.3587	5.87597	0.00481
H	-2.10433	4.99502	-1.30707
C	2.26777	3.68636	-2.73664
H	2.17003	4.74951	-2.80774
H	3.04496	3.44532	-2.04181
H	2.51206	3.28554	-3.69818
C	1.72471	-4.92089	-0.30943
H	2.50796	-4.60526	0.34769
H	1.3587	-5.87597	0.00481
H	2.10433	-4.99502	-1.30707
C	-2.26777	-3.68636	-2.73664
H	-3.04496	-3.44532	-2.04181
H	-2.51206	-3.28554	-3.69818
H	-2.17003	-4.74951	-2.80774

**(P<sub>2</sub>)-DESp**

C	-0.30442	1.15663	6.18146
C	-0.29262	1.10998	4.78334
C	0.	0.	6.88314
C	0.30442	-1.15663	6.18146
H	0.54707	-2.08282	6.68932
C	0.29262	-1.10998	4.78334
H	0.	0.	7.96859
N	0.	0.	4.09672
H	-0.54707	2.08282	6.68932

C	3.56644	8.51724	0.06865
C	3.58489	7.38648	-0.74098
C	2.40406	6.67655	-0.92542
C	1.21912	7.09625	-0.309
C	1.20114	8.22252	0.49527
C	2.3859	8.93074	0.68394
H	4.48048	9.0817	0.22483
H	4.50742	7.06493	-1.2153
H	0.28103	8.54827	0.97125
H	2.38922	9.81352	1.31567
C	0.05575	6.18512	-0.69736
C	0.77092	5.1298	-1.53206
C	0.25912	3.95602	-2.04499
C	2.12818	5.44688	-1.67776
C	1.11984	3.07161	-2.71611
H	-0.77952	3.68162	-1.89418
C	2.97298	4.60425	-2.39176
C	2.46595	3.42003	-2.90731
H	4.02417	4.84519	-2.51741
H	3.11723	2.72932	-3.43164
C	-0.73961	5.61225	0.47071
C	-0.32832	4.70222	1.4249
C	-2.06117	6.07735	0.44435
C	-1.25231	4.25006	2.37991
H	0.68104	4.30437	1.42479
C	-2.96895	5.66847	1.41428
C	-2.55991	4.75864	2.37857
H	-3.99323	6.0286	1.40626
H	-3.26144	4.40247	3.12508
C	-1.02571	6.96851	-1.44012
C	-2.23638	6.9276	-0.73924
C	-0.91615	7.68099	-2.62174
C	-3.3521	7.60428	-1.21837
C	-2.03576	8.35495	-3.10431
H	0.02433	7.7136	-3.16365
C	-3.24218	8.31844	-2.40681
H	-4.29472	7.57491	-0.6798
H	-1.96758	8.91416	-4.0322
H	-4.10462	8.85054	-2.79612
C	-0.89096	3.21156	3.29555
C	-0.60993	2.2735	4.00187
C	0.64457	1.77656	-3.07873
C	0.23124	0.64394	-3.2039
C	3.24218	-8.31844	-2.40681
C	3.3521	-7.60428	-1.21837
C	2.23638	-6.9276	-0.73924
C	1.02571	-6.96851	-1.44012
C	0.91615	-7.68099	-2.62174
C	2.03576	-8.35495	-3.10431
H	4.10462	-8.85054	-2.79612
H	4.29472	-7.57491	-0.6798
H	-0.02433	-7.7136	-3.16365
H	1.96758	-8.91416	-4.0322
C	-0.05575	-6.18512	-0.69736
C	0.73961	-5.61225	0.47071
C	0.32832	-4.70222	1.4249

C	2.06117	-6.07735	0.44435
C	1.25231	-4.25006	2.37991
H	-0.68104	-4.30437	1.42479
C	2.96895	-5.66847	1.41428
C	2.55991	-4.75864	2.37857
H	3.99323	-6.0286	1.40626
H	3.26144	-4.40247	3.12508
C	-0.77092	-5.1298	-1.53206
C	-0.25912	-3.95602	-2.04499
C	-2.12818	-5.44688	-1.67776
C	-1.11984	-3.07161	-2.71611
H	0.77952	-3.68162	-1.89418
C	-2.97298	-4.60425	-2.39176
C	-2.46595	-3.42003	-2.90731
H	-4.02417	-4.84519	-2.51741
H	-3.11723	-2.72932	-3.43164
C	-1.21912	-7.09625	-0.309
C	-2.40406	-6.67655	-0.92542
C	-1.20114	-8.22252	0.49527
C	-3.58489	-7.38648	-0.74098
C	-2.3859	-8.93074	0.68394
H	-0.28103	-8.54827	0.97125
C	-3.56644	-8.51724	0.06865
H	-4.50742	-7.06493	-1.2153
H	-2.38922	-9.81352	1.31567
H	-4.48048	-9.0817	0.22483
C	-0.64457	-1.77656	-3.07873
C	-0.23124	-0.64394	-3.2039
C	0.89096	-3.21156	3.29555
C	0.60993	-2.2735	4.00187

**(P<sub>2</sub>)-DEAbp**

C	0.06489	2.7052	2.21696
C	0.11007	0.75604	3.42987
C	0.54732	1.4299	4.57329
C	0.73525	2.8033	4.50787
C	0.49037	3.46173	3.31351
H	0.75937	0.8866	5.48729
H	1.08012	3.35286	5.37818
H	0.62802	4.5322	3.21397
C	-0.11007	-0.75604	3.42987
C	-0.54732	-1.4299	4.57329
C	-0.73525	-2.8033	4.50787
H	-0.75937	-0.8866	5.48729
C	-0.06489	-2.7052	2.21696
C	-0.49037	-3.46173	3.31351
H	-1.08012	-3.35286	5.37818
H	-0.62802	-4.5322	3.21397
N	-0.1244	1.38283	2.27844
N	0.1244	-1.38283	2.27844
C	-0.19036	3.32265	0.94423
C	-0.40531	3.76642	-0.15767
C	0.19036	-3.32265	0.94423
C	0.40531	-3.76642	-0.15767



C	-0.72567	4.18099	-1.49395
C	0.72567	-4.18099	-1.49395
C	0.01563	3.73733	-2.48202
C	-0.01563	-3.73733	-2.48202
C	0.74234	3.17149	-3.41963
C	-0.74234	-3.17149	-3.41963
C	0.41104	1.8242	-3.77349
C	0.14837	0.64909	-3.90891
C	-0.41104	-1.8242	-3.77349
C	-0.14837	-0.64909	-3.90891
C	-1.95083	5.04436	-1.69978
H	-2.8368	4.54493	-1.29609
H	-1.83969	5.99825	-1.17445
H	-2.10965	5.24338	-2.76116
C	1.94116	3.82733	-4.06614
H	2.83908	3.22438	-3.90029
H	1.79409	3.91226	-5.14742
H	2.10417	4.82484	-3.65397
C	-1.94116	-3.82733	-4.06614
H	-2.83908	-3.22438	-3.90029
H	-1.79409	-3.91226	-5.14742
H	-2.10417	-4.82484	-3.65397
C	1.95083	-5.04436	-1.69978
H	2.8368	-4.54493	-1.29609
H	1.83969	-5.99825	-1.17445
H	2.10965	-5.24338	-2.76116

**(P<sub>2</sub>)-DESbp**

C	0.10236	2.73352	5.1255
C	0.16292	0.72897	6.23338
C	0.78207	1.30874	7.34245
C	1.07499	2.66456	7.30997
C	0.73089	3.39632	6.18581
H	1.04701	0.69979	8.19989
H	1.56845	3.14351	8.14994
H	0.93249	4.45873	6.1135
C	-0.16292	-0.72897	6.23338
C	-0.78207	-1.30874	7.34245
C	-1.07499	-2.66456	7.30997
H	-1.04701	-0.69979	8.19989
C	-0.10236	-2.73352	5.1255
C	-0.73089	-3.39632	6.18581
H	-1.56845	-3.14351	8.14994
H	-0.93249	-4.45873	6.1135
N	-0.16891	1.42319	5.14546
N	0.16891	-1.42319	5.14546
C	3.41868	8.91282	-1.08745
C	3.47705	7.67997	-1.72873
C	2.32101	6.91202	-1.80858
C	1.1208	7.37506	-1.2545
C	1.06373	8.60265	-0.61753
C	2.22342	9.37016	-0.53474
H	4.31285	9.5242	-1.01519
H	4.41087	7.32585	-2.15538

H	0.13209	8.96105	-0.18992
H	2.19573	10.33381	-0.03572
C	-0.00674	6.37592	-1.49472
C	0.73944	5.24821	-2.1983
C	0.25344	4.01652	-2.58318
C	2.08539	5.58495	-2.39045
C	1.12996	3.09094	-3.17206
H	-0.78034	3.73897	-2.40657
C	2.95013	4.68843	-3.00916
C	2.46955	3.44576	-3.39674
H	3.99404	4.94089	-3.1684
H	3.13403	2.7215	-3.85507
C	-0.75062	5.91789	-0.24447
C	-0.24974	5.24798	0.85527
C	-2.11507	6.21905	-0.34368
C	-1.1293	4.8654	1.8789
H	0.80313	4.99612	0.92837
C	-2.9891	5.85985	0.67569
C	-2.49277	5.18364	1.78021
H	-4.04844	6.08811	0.6079
H	-3.15937	4.87892	2.57951
C	-1.14493	6.96993	-2.32148
C	-2.35857	6.88169	-1.63052
C	-1.08682	7.54636	-3.57863
C	-3.52963	7.37266	-2.1963
C	-2.26062	8.03679	-4.14613
H	-0.14409	7.61497	-4.11327
C	-3.47096	7.95118	-3.45974
H	-4.47464	7.3061	-1.66527
H	-2.2324	8.48982	-5.1322
H	-4.37638	8.33876	-3.91638
C	-0.65931	4.12795	3.01182
C	-0.30295	3.47563	3.96317
C	0.6658	1.77137	-3.44771
C	0.23746	0.64154	-3.54135
C	3.47096	-7.95118	-3.45974
C	3.52963	-7.37266	-2.1963
C	2.35857	-6.88169	-1.63052
C	1.14493	-6.96993	-2.32148
C	1.08682	-7.54636	-3.57863
C	2.26062	-8.03679	-4.14613
H	4.37638	-8.33876	-3.91638
H	4.47464	-7.3061	-1.66527
H	0.14409	-7.61497	-4.11327
H	2.2324	-8.48982	-5.1322
C	0.00674	-6.37592	-1.49472
C	0.75062	-5.91789	-0.24447
C	0.24974	-5.24798	0.85527
C	2.11507	-6.21905	-0.34368
C	1.1293	-4.8654	1.8789
H	-0.80313	-4.99612	0.92837
C	2.9891	-5.85985	0.67569
C	2.49277	-5.18364	1.78021
H	4.04844	-6.08811	0.6079
H	3.15937	-4.87892	2.57951
C	-0.73944	-5.24821	-2.1983

C	-0.25344	-4.01652	-2.58318
C	-2.08539	-5.58495	-2.39045
C	-1.12996	-3.09094	-3.17206
H	0.78034	-3.73897	-2.40657
C	-2.95013	-4.68843	-3.00916
C	-2.46955	-3.44576	-3.39674
H	-3.99404	-4.94089	-3.1684
H	-3.13403	-2.7215	-3.85507
C	-1.1208	-7.37506	-1.2545
C	-2.32101	-6.91202	-1.80858
C	-1.06373	-8.60265	-0.61753
C	-3.47705	-7.67997	-1.72873
C	-2.22342	-9.37016	-0.53474
H	-0.13209	-8.96105	-0.18992
C	-3.41868	-8.91282	-1.08745
H	-4.41087	-7.32585	-2.15538
H	-2.19573	-10.33381	-0.03572
H	-4.31285	-9.5242	-1.01519
C	-0.6658	-1.77137	-3.44771
C	-0.23746	-0.64154	-3.54135
C	0.65931	-4.12795	3.01182
C	0.30295	-3.47563	3.96317

**(P)-DEA**

C	-4.61525	-1.496	-0.02125
H	-5.68525	-1.496	-0.02125
C	-3.41405	-1.496	-0.02125
C	-1.87405	-1.496	-0.02125
C	-1.1918	-2.53359	0.52144
C	-0.50956	-3.57118	1.06414
C	-0.10899	-4.77011	0.18453
C	0.20346	-5.70528	-0.50157
H	0.48177	-6.5383	-1.11273
C	-0.13348	-3.55545	2.55743
H	-0.91423	-4.01504	3.12672
H	0.77853	-4.09624	2.70126
H	-0.00343	-2.54414	2.88184
C	-1.10669	-0.31286	-0.64008
H	-0.7762	-0.57701	-1.62288
H	-1.75117	0.53933	-0.69753
H	-0.25952	-0.07887	-0.02978

**(P)-DES**

C	7.89872	2.90281	2.11261
C	8.06339	4.23632	2.45603
C	7.87529	5.21239	1.48362
C	7.51976	4.8498	0.17809
C	7.35495	3.52512	-0.17165
C	7.54764	2.53335	0.80367
H	8.04289	2.12519	2.85464
H	8.33735	4.50666	3.47126

H	7.08294	3.23953	-1.18243
C	7.37016	6.08621	-0.70337
C	7.70045	7.20041	0.28433
C	7.73583	8.56642	0.0625
C	7.98732	6.67422	1.54966
C	8.0619	9.40968	1.12225
H	7.51332	8.97391	-0.91916
C	8.31263	7.51604	2.60705
C	8.3475	8.88819	2.38321
H	8.09326	10.48322	0.96462
H	8.53549	7.11341	3.59074
H	8.59909	9.55985	3.1981
C	8.26421	6.06659	-1.93868
C	9.64326	5.96433	-2.00266
C	7.49975	6.16686	-3.10741
C	10.25824	5.96265	-3.25259
H	10.23527	5.88664	-1.09564
C	8.1138	6.16488	-4.35464
C	9.49929	6.06178	-4.4178
H	11.3387	5.88276	-3.3198
H	7.52593	6.24181	-5.26451
H	9.99478	6.05817	-5.3837
C	5.98801	6.22159	-1.33538
C	6.08419	6.26398	-2.73228
C	4.76354	6.30413	-0.7046
C	4.93831	6.38566	-3.51073
C	3.60216	6.43181	-1.48378
H	4.68437	6.275	0.37711
C	3.70383	6.46889	-2.88426
H	5.00148	6.41745	-4.59416
C	2.32614	6.53179	-0.85675
H	2.79772	6.56621	-3.47211
C	7.39686	1.15652	0.46649
C	1.25583	6.6255	-0.31958
H	0.30243	6.70898	0.15892
C	7.27912	-0.00254	0.17391
H	7.17424	-1.035	-0.08672

# M062X/6-31G\* XYZ geometries ( Å ):

## (P<sub>4</sub>)-DEA

C	-0.66932	4.91488	0.144
C	0.66932	4.91488	-0.144
C	-1.8539	4.87186	0.39296
C	1.8539	4.87186	-0.39296
C	-3.2418	4.78599	0.72895
C	-4.03105	4.03105	0.
C	3.2418	4.78599	-0.72895
C	4.03105	4.03105	0.
C	-4.78599	3.2418	-0.72895
C	4.78599	3.2418	0.72895
C	-4.87186	1.8539	-0.39296
C	-4.91488	0.66932	-0.144
C	4.87186	1.8539	0.39296
C	4.91488	0.66932	0.144
C	-4.91488	-0.66932	0.144
C	-4.87186	-1.8539	0.39296
C	-4.78599	-3.2418	0.72895
C	-4.03105	-4.03105	0.
C	-3.2418	-4.78599	-0.72895
C	-1.8539	-4.87186	-0.39296
C	-0.66932	-4.91488	-0.144
C	0.66932	-4.91488	0.144
C	1.8539	-4.87186	0.39296
C	3.2418	-4.78599	0.72895
C	4.03105	-4.03105	0.
C	4.78599	-3.2418	-0.72895
C	4.87186	-1.8539	-0.39296
C	4.91488	-0.66932	-0.144
C	-5.55695	-3.72875	1.9383
H	-5.24073	-3.18366	2.8327
H	-6.62849	-3.55253	1.80328
H	-5.39081	-4.79562	2.09753
C	-3.72875	-5.55695	-1.9383
H	-3.18366	-5.24073	-2.8327
H	-3.55253	-6.62849	-1.80328
H	-4.79562	-5.39081	-2.09753
C	5.55695	-3.72875	-1.9383
H	5.24073	-3.18366	-2.8327
H	6.62849	-3.55253	-1.80328
H	5.39081	-4.79562	-2.09753
C	3.72875	-5.55695	1.9383
H	3.18366	-5.24073	2.8327
H	3.55253	-6.62849	1.80328
H	4.79562	-5.39081	2.09753
C	-3.72875	5.55695	1.9383
H	-3.18366	5.24073	2.8327
H	-3.55253	6.62849	1.80328
H	-4.79562	5.39081	2.09753
C	-5.55695	3.72875	-1.9383
H	-5.24073	3.18366	-2.8327

H	-6.62849	3.55253	-1.80328
H	-5.39081	4.79562	-2.09753
C	3.72875	5.55695	-1.9383
H	3.18366	5.24073	-2.8327
H	3.55253	6.62849	-1.80328
H	4.79562	5.39081	-2.09753
C	5.55695	3.72875	1.9383
H	5.24073	3.18366	2.8327
H	6.62849	3.55253	1.80328
H	5.39081	4.79562	2.09753

**(P<sub>4</sub>)-DES**

**(P<sub>2</sub>)-DEAp**

C	0.10897	-1.19484	4.05269
C	0.	0.	4.75095
H	0.19496	-2.14605	4.56524
C	-0.10616	1.14632	2.65567
C	-0.10897	1.19484	4.05269
H	0.	0.	5.83641
H	-0.19496	2.14605	4.56524
N	0.	0.	1.976
C	-0.22898	2.31121	1.82125
C	-0.35198	3.11865	0.93092
C	-0.56229	3.89693	-0.2572
C	0.17952	3.58875	-1.2975
C	0.90796	3.08762	-2.27085
C	0.49338	1.8152	-2.78478
C	0.10616	-1.14632	2.65567
C	0.22898	-2.31121	1.82125
C	0.35198	-3.11865	0.93092
C	0.56229	-3.89693	-0.2572
C	-0.17952	-3.58875	-1.2975
C	-0.90796	-3.08762	-2.27085
C	-0.49338	-1.8152	-2.78478
C	-0.17791	-0.6615	-2.98418
C	0.17791	0.6615	-2.98418
C	-1.68492	4.90735	-0.28802
H	-2.63339	4.42962	-0.02418
H	-1.50249	5.70525	0.43889
H	-1.7769	5.35228	-1.28047
C	2.1992	3.6984	-2.76282
H	2.42928	4.6114	-2.21054
H	3.02464	2.99087	-2.63926
H	2.12692	3.94066	-3.8278
C	1.68492	-4.90735	-0.28802
H	2.63339	-4.42962	-0.02418
H	1.50249	-5.70525	0.43889
H	1.7769	-5.35228	-1.28047
C	-2.1992	-3.6984	-2.76282
H	-3.02464	-2.99087	-2.63926
H	-2.12692	-3.94066	-3.8278
H	-2.42928	-4.6114	-2.21054

**(P<sub>2</sub>)-DESp**

C	-0.30431	1.15663	6.18103
C	-0.29256	1.11004	4.7829
C	0.	0.	6.8827
C	0.30431	-1.15663	6.18103
H	0.54685	-2.08284	6.6889
C	0.29256	-1.11004	4.7829
H	0.	0.	7.96815
N	0.	0.	4.0962
H	-0.54685	2.08284	6.6889
C	3.56686	8.5174	0.06743
C	3.58495	7.38675	-0.74223
C	2.40394	6.67688	-0.92625
C	1.21926	7.09663	-0.30935
C	1.20171	8.22287	0.49503
C	2.38654	8.93094	0.68323
H	4.48087	9.08198	0.22341
H	4.5072	7.06502	-1.21696
H	0.28174	8.5485	0.97137
H	2.3904	9.81371	1.31497
C	0.05579	6.18546	-0.69737
C	0.77057	5.13019	-1.53225
C	0.25867	3.95632	-2.04495
C	2.12779	5.44729	-1.67846
C	1.11911	3.07188	-2.71624
H	-0.78002	3.68222	-1.89389
C	2.97235	4.60466	-2.39283
C	2.46521	3.42039	-2.908
H	4.02342	4.84589	-2.51899
H	3.11615	2.72964	-3.43268
C	-0.73919	5.61292	0.47098
C	-0.32787	4.70269	1.42505
C	-2.0606	6.07849	0.4452
C	-1.25154	4.25088	2.38045
H	0.68148	4.30481	1.42449
C	-2.9681	5.67	1.41562
C	-2.55901	4.76002	2.37965
H	-3.99214	6.03081	1.40807
H	-3.26018	4.40419	3.12666
C	-1.02572	6.96908	-1.43985
C	-2.23607	6.92863	-0.73833
C	-0.91659	7.68133	-2.62168
C	-3.35186	7.60562	-1.21702
C	-2.03621	8.35551	-3.10371
H	0.02366	7.71342	-3.16401
C	-3.24232	8.31951	-2.40556
H	-4.29415	7.57652	-0.67785
H	-1.96859	8.91459	-4.03172
H	-4.10466	8.85192	-2.79469
C	-0.8905	3.21208	3.29577
C	-0.6097	2.2736	4.00168
C	0.6442	1.77665	-3.07842
C	0.23108	0.644	-3.20421

C	3.24232	-8.31951	-2.40556
C	3.35186	-7.60562	-1.21702
C	2.23607	-6.92863	-0.73833
C	1.02572	-6.96908	-1.43985
C	0.91659	-7.68133	-2.62168
C	2.03621	-8.35551	-3.10371
H	4.10466	-8.85192	-2.79469
H	4.29415	-7.57652	-0.67785
H	-0.02366	-7.71342	-3.16401
H	1.96859	-8.91459	-4.03172
C	-0.05579	-6.18546	-0.69737
C	0.73919	-5.61292	0.47098
C	0.32787	-4.70269	1.42505
C	2.0606	-6.07849	0.4452
C	1.25154	-4.25088	2.38045
H	-0.68148	-4.30481	1.42449
C	2.9681	-5.67	1.41562
C	2.55901	-4.76002	2.37965
H	3.99214	-6.03081	1.40807
H	3.26018	-4.40419	3.12666
C	-0.77057	-5.13019	-1.53225
C	-0.25867	-3.95632	-2.04495
C	-2.12779	-5.44729	-1.67846
C	-1.11911	-3.07188	-2.71624
H	0.78002	-3.68222	-1.89389
C	-2.97235	-4.60466	-2.39283
C	-2.46521	-3.42039	-2.908
H	-4.02342	-4.84589	-2.51899
H	-3.11615	-2.72964	-3.43268
C	-1.21926	-7.09663	-0.30935
C	-2.40394	-6.67688	-0.92625
C	-1.20171	-8.22287	0.49503
C	-3.58495	-7.38675	-0.74223
C	-2.38654	-8.93094	0.68323
H	-0.28174	-8.5485	0.97137
C	-3.56686	-8.5174	0.06743
H	-4.5072	-7.06502	-1.21696
H	-2.3904	-9.81371	1.31497
H	-4.48087	-9.08198	0.22341
C	-0.6442	-1.77665	-3.07842
C	-0.23108	-0.644	-3.20421
C	0.8905	-3.21208	3.29577
C	0.6097	-2.2736	4.00168

**(P<sub>2</sub>)-DEAbp**

C	0.06639	2.69455	2.21567
C	0.11069	0.73933	3.41878
C	0.54951	1.40699	4.56526
C	0.73892	2.78048	4.50651
C	0.49376	3.44505	3.31559
H	0.76155	0.85886	5.47637
H	1.08514	3.32541	5.37918
H	0.63257	4.51584	3.22124
C	-0.11069	-0.73933	3.41878



C	-0.54951	-1.40699	4.56526
C	-0.73892	-2.78048	4.50651
H	-0.76155	-0.85886	5.47637
C	-0.06639	-2.69455	2.21567
C	-0.49376	-3.44505	3.31559
H	-1.08514	-3.32541	5.37918
H	-0.63257	-4.51584	3.22124
N	-0.12422	1.372	2.27072
N	0.12422	-1.372	2.27072
C	-0.18947	3.31878	0.94643
C	-0.40521	3.76869	-0.15283
C	0.18947	-3.31878	0.94643
C	0.40521	-3.76869	-0.15283
C	-0.72618	4.19005	-1.48686
C	0.72618	-4.19005	-1.48686
C	0.01428	3.75059	-2.47745
C	-0.01428	-3.75059	-2.47745
C	0.74002	3.18858	-3.41813
C	-0.74002	-3.18858	-3.41813
C	0.40761	1.84325	-3.77798
C	0.14825	0.66835	-3.92095
C	-0.40761	-1.84325	-3.77798
C	-0.14825	-0.66835	-3.92095
C	-1.95099	5.05505	-1.68767
H	-2.83691	4.55417	-1.28571
H	-1.83886	6.00635	-1.15791
H	-2.11041	5.25915	-2.74799
C	1.93915	3.84646	-4.06192
H	2.83652	3.24186	-3.8993
H	1.79172	3.93674	-5.1427
H	2.10304	4.84181	-3.64492
C	-1.93915	-3.84646	-4.06192
H	-2.83652	-3.24186	-3.8993
H	-1.79172	-3.93674	-5.1427
H	-2.10304	-4.84181	-3.64492
C	1.95099	-5.05505	-1.68767
H	2.83691	-4.55417	-1.28571
H	1.83886	-6.00635	-1.15791
H	2.11041	-5.25915	-2.74799

**(P<sub>2</sub>)-DESbp**

C	0.10226	2.7335	5.12554
C	0.16288	0.72898	6.23343
C	0.78187	1.30882	7.34257
C	1.07468	2.66465	7.31011
C	0.73061	3.39637	6.18591
H	1.04679	0.69989	8.20002
H	1.56801	3.14365	8.15011
H	0.93209	4.4588	6.11361
C	-0.16288	-0.72898	6.23343
C	-0.78187	-1.30882	7.34257
C	-1.07468	-2.66465	7.31011
H	-1.04679	-0.69989	8.20002
C	-0.10226	-2.7335	5.12554

C	-0.73061	-3.39637	6.18591
H	-1.56801	-3.14365	8.15011
H	-0.93209	-4.4588	6.11361
N	-0.16891	1.42316	5.14549
N	0.16891	-1.42316	5.14549
C	3.41872	8.91279	-1.0874
C	3.47706	7.67996	-1.72872
C	2.32102	6.91203	-1.80858
C	1.12083	7.37506	-1.25448
C	1.06378	8.60262	-0.61747
C	2.22348	9.37012	-0.53466
H	4.31291	9.52415	-1.01515
H	4.41088	7.32586	-2.15539
H	0.13216	8.96103	-0.18983
H	2.19578	10.33375	-0.0356
C	-0.00673	6.37594	-1.49471
C	0.73944	5.24823	-2.19832
C	0.25343	4.01654	-2.58318
C	2.08538	5.58497	-2.39049
C	1.12995	3.09096	-3.17205
H	-0.78033	3.73896	-2.40653
C	2.9501	4.68845	-3.00922
C	2.46952	3.44578	-3.3968
H	3.99401	4.9409	-3.16848
H	3.134	2.72152	-3.85513
C	-0.75065	5.91786	-0.24448
C	-0.24978	5.24796	0.85526
C	-2.1151	6.21896	-0.34375
C	-1.12937	4.86532	1.87886
H	0.80308	4.99612	0.92842
C	-2.98915	5.85969	0.67558
C	-2.49284	5.18349	1.78011
H	-4.0485	6.08788	0.60775
H	-3.15947	4.87872	2.57936
C	-1.14492	6.96995	-2.32147
C	-2.35859	6.88162	-1.63058
C	-1.08677	7.54643	-3.57859
C	-3.52965	7.37252	-2.19641
C	-2.26058	8.03682	-4.14614
H	-0.14403	7.61514	-4.11319
C	-3.47094	7.9511	-3.45982
H	-4.47468	7.3059	-1.66544
H	-2.2323	8.4899	-5.13219
H	-4.37638	8.33864	-3.91648
C	-0.65935	4.12787	3.01178
C	-0.30301	3.47557	3.96315
C	0.66578	1.77137	-3.44767
C	0.23746	0.64154	-3.54136
C	3.47094	-7.9511	-3.45982
C	3.52965	-7.37252	-2.19641
C	2.35859	-6.88162	-1.63058
C	1.14492	-6.96995	-2.32147
C	1.08677	-7.54643	-3.57859
C	2.26058	-8.03682	-4.14614
H	4.37638	-8.33864	-3.91648
H	4.47468	-7.3059	-1.66544

H	0.14403	-7.61514	-4.11319
H	2.2323	-8.4899	-5.13219
C	0.00673	-6.37594	-1.49471
C	0.75065	-5.91786	-0.24448
C	0.24978	-5.24796	0.85526
C	2.1151	-6.21896	-0.34375
C	1.12937	-4.86532	1.87886
H	-0.80308	-4.99612	0.92842
C	2.98915	-5.85969	0.67558
C	2.49284	-5.18349	1.78011
H	4.0485	-6.08788	0.60775
H	3.15947	-4.87872	2.57936
C	-0.73944	-5.24823	-2.19832
C	-0.25343	-4.01654	-2.58318
C	-2.08538	-5.58497	-2.39049
C	-1.12995	-3.09096	-3.17205
H	0.78033	-3.73896	-2.40653
C	-2.9501	-4.68845	-3.00922
C	-2.46952	-3.44578	-3.3968
H	-3.99401	-4.9409	-3.16848
H	-3.134	-2.72152	-3.85513
C	-1.12083	-7.37506	-1.25448
C	-2.32102	-6.91203	-1.80858
C	-1.06378	-8.60262	-0.61747
C	-3.47706	-7.67996	-1.72872
C	-2.22348	-9.37012	-0.53466
H	-0.13216	-8.96103	-0.18983
C	-3.41872	-8.91279	-1.0874
H	-4.41088	-7.32586	-2.15539
H	-2.19578	-10.33375	-0.0356
H	-4.31291	-9.52415	-1.01515
C	-0.66578	-1.77137	-3.44767
C	-0.23746	-0.64154	-3.54136
C	0.65935	-4.12787	3.01178
C	0.30301	-3.47557	3.96315

**(P)-DEA**

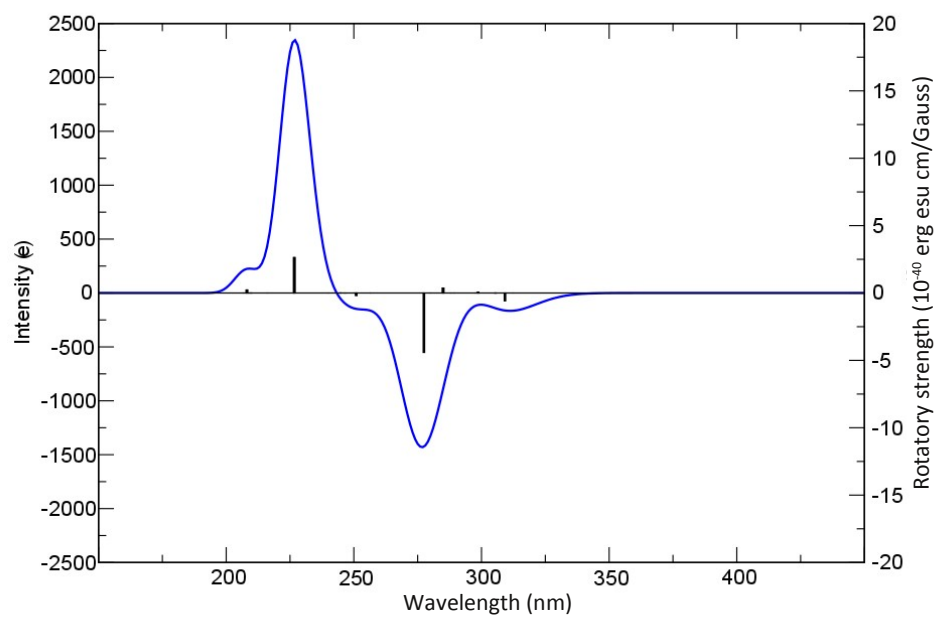
C	0.93918	2.9771	1.32409
H	1.43782	3.66784	1.96529
C	0.38392	2.18451	0.60826
C	-0.30396	1.27601	-0.26487
C	0.	0.	-0.26376
C	0.30396	-1.27601	-0.26487
C	-0.38392	-2.18451	0.60826
C	-0.93918	-2.9771	1.32409
H	-1.43782	-3.66784	1.96529
C	1.37318	-1.85553	-1.16751
H	2.15503	-2.33331	-0.56926
H	0.9446	-2.62006	-1.8229
H	1.82614	-1.07532	-1.78167
C	-1.37318	1.85553	-1.16751
H	-2.15503	2.33331	-0.56926
H	-0.9446	2.62006	-1.8229
H	-1.82614	1.07532	-1.78167

**(P)-DES**

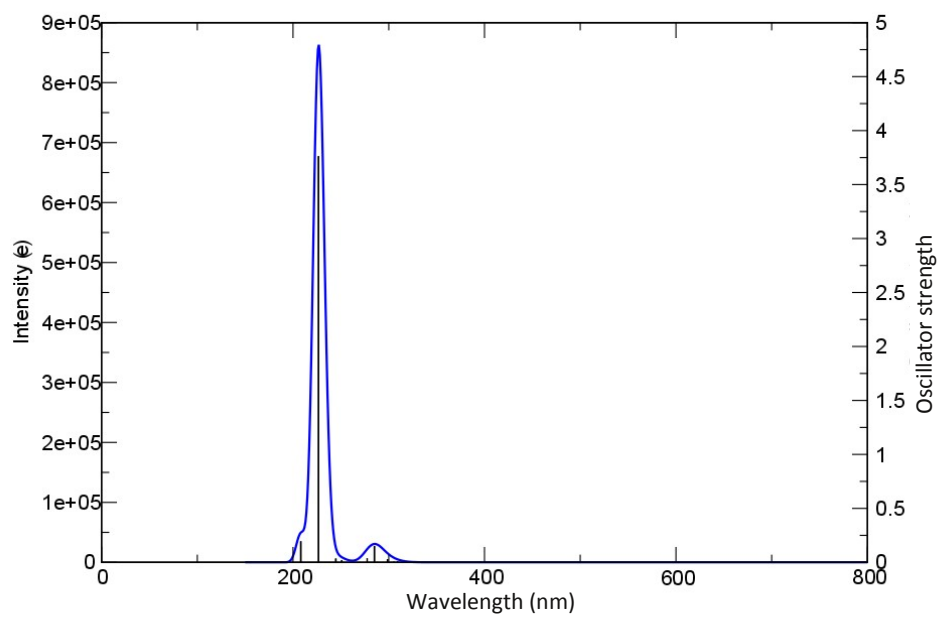
C	-0.33144	3.70636	1.61445
C	-1.25324	3.31114	0.65559
C	-1.07643	2.09177	0.0118
C	0.01759	1.27744	0.33004
C	0.93826	1.66523	1.2831
C	0.76616	2.89419	1.93641
H	-0.45031	4.65364	2.12898
H	-2.09806	3.95006	0.41702
H	1.78752	1.03759	1.53239
C	0.	0.	-0.50363
C	-1.26065	0.20362	-1.338
C	-1.80638	-0.63629	-2.29356
C	-1.87183	1.42374	-1.02575
C	-2.97662	-0.24542	-2.94021
H	-1.33162	-1.58266	-2.53485
C	-3.03952	1.81367	-1.67138
C	-3.58713	0.96918	-2.63129
H	-3.41749	-0.89306	-3.69156
H	-3.51825	2.7589	-1.43302
H	-4.49893	1.25828	-3.14464
C	1.26065	-0.20362	-1.338
C	1.80638	0.63629	-2.29356
C	1.87183	-1.42374	-1.02575
C	2.97662	0.24542	-2.94021
H	1.33162	1.58266	-2.53485
C	3.03952	-1.81367	-1.67138
C	3.58713	-0.96918	-2.63129
H	3.41749	0.89306	-3.69156
H	3.51825	-2.7589	-1.43302
H	4.49893	-1.25828	-3.14464
C	-0.01759	-1.27744	0.33004
C	1.07643	-2.09177	0.0118
C	-0.93826	-1.66523	1.2831
C	1.25324	-3.31114	0.65559
C	-0.76616	-2.89419	1.93641
H	-1.78752	-1.03759	1.53239
C	0.33144	-3.70636	1.61445
H	2.09806	-3.95006	0.41702
C	-1.70662	-3.31995	2.92864
H	0.45031	-4.65364	2.12898
C	1.70662	3.31995	2.92864
C	-2.49737	-3.67843	3.76262
H	-3.19789	-3.99424	4.50183
C	2.49737	3.67843	3.76262
H	3.19789	3.99424	4.50183

## CAMB3LYP ECD and UV

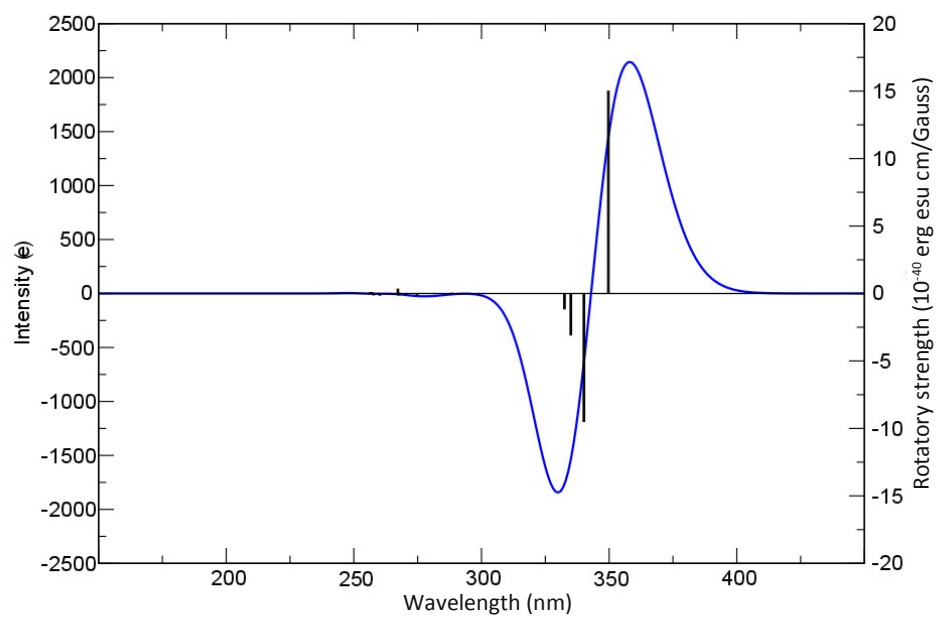
(*P*<sub>4</sub>)-DEA-ECD



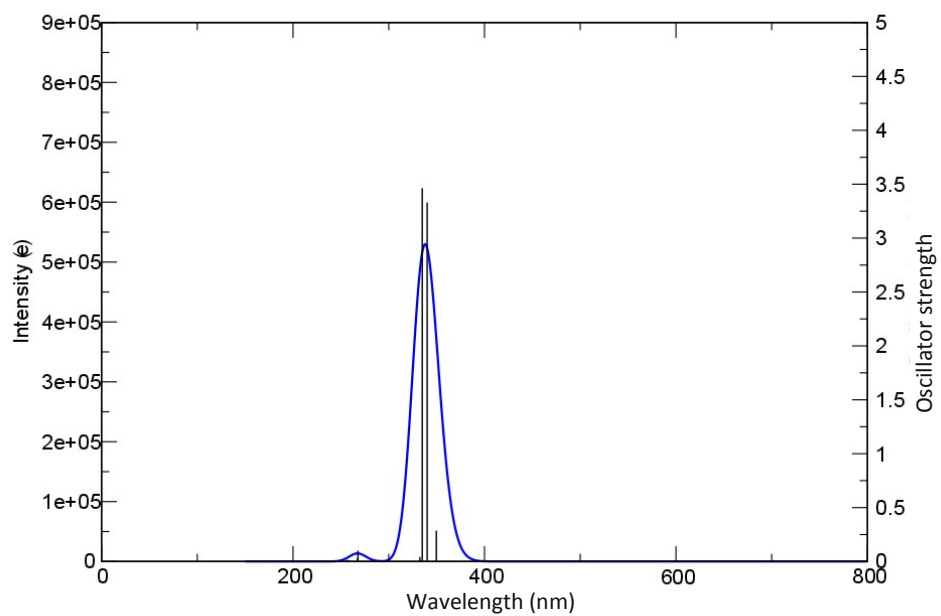
(*P*<sub>4</sub>)-DEA-UV



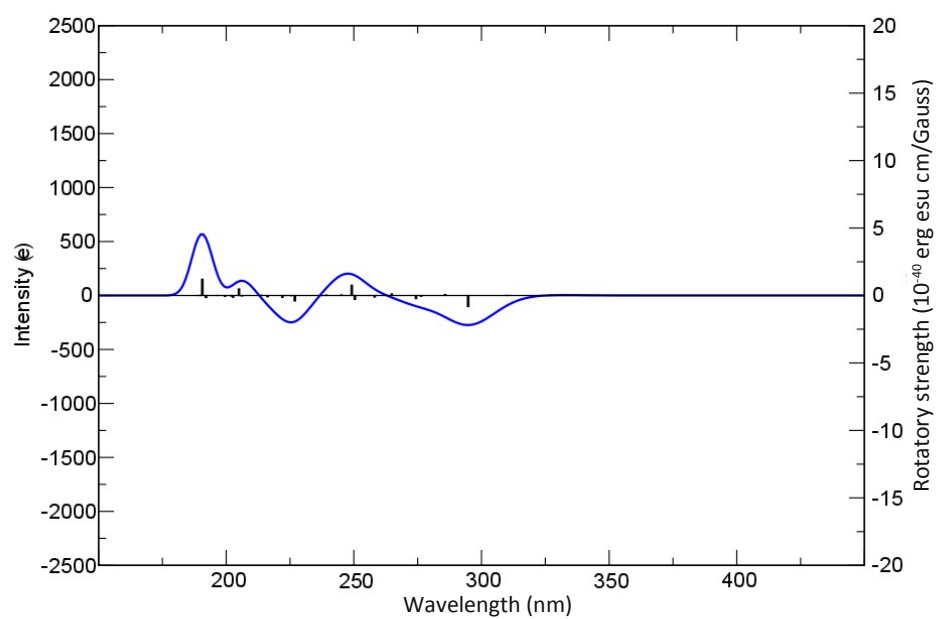
**$(P_4)$ -DES-ECD**



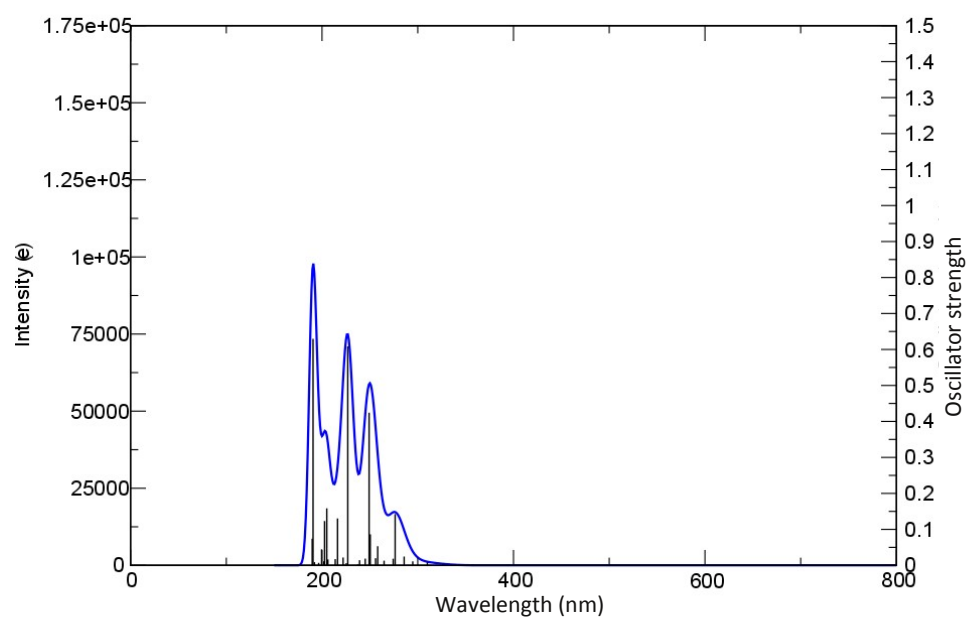
**$(P_4)$ -DES-UV**



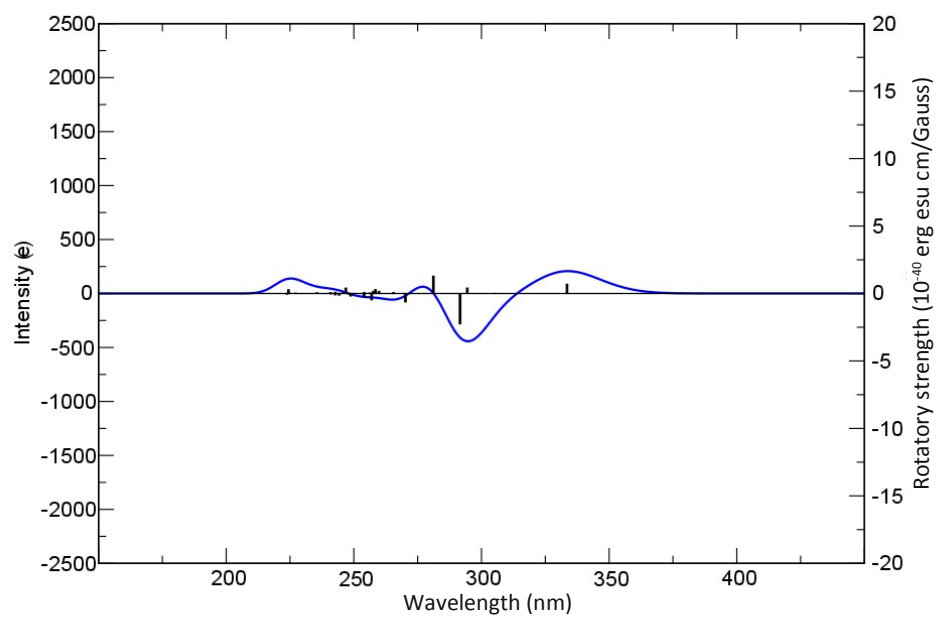
**$(P_2)$ -DEAp-ECD**



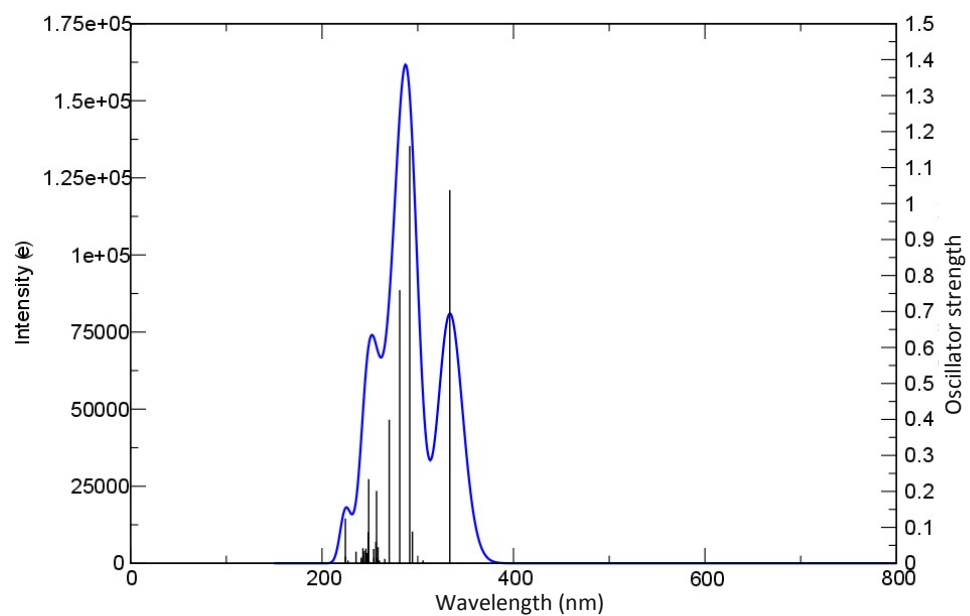
**$(P_2)$ -DEAp-UV**



**$(P_2)$ -DESp-ECD**

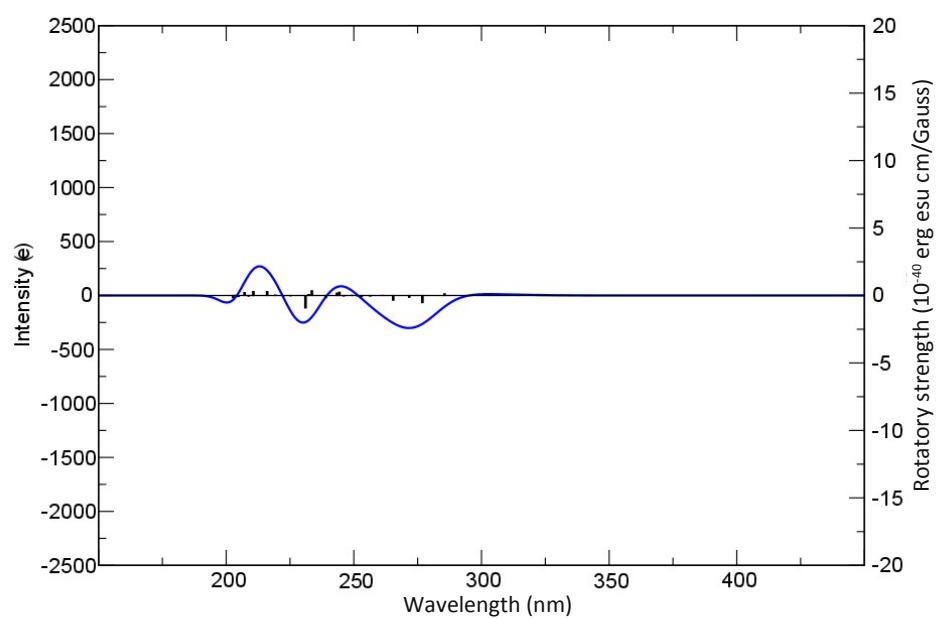


**$(P_2)$ -DESp-UV**

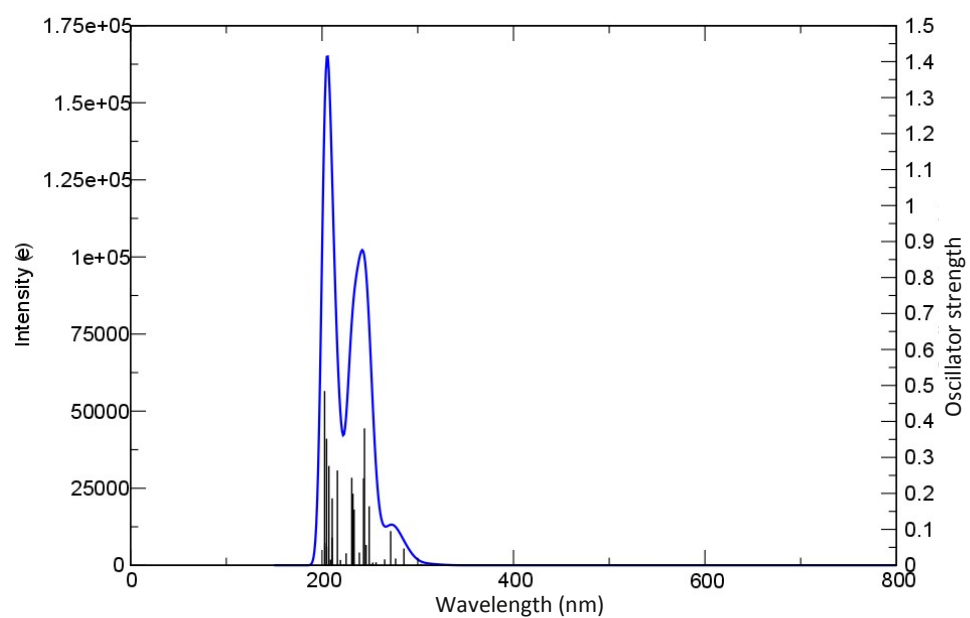




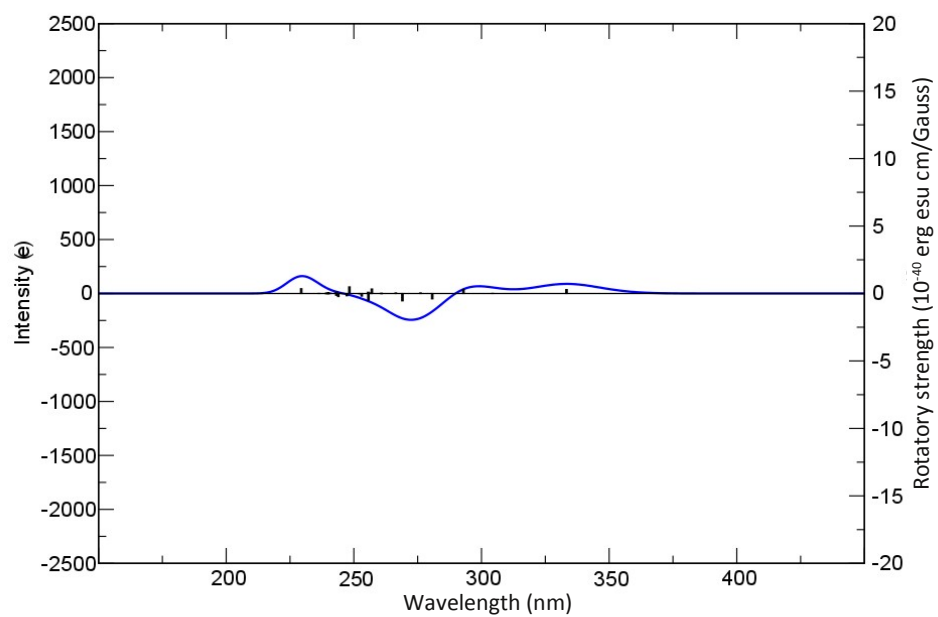
**(P<sub>2</sub>)-DEAbp-ECD**



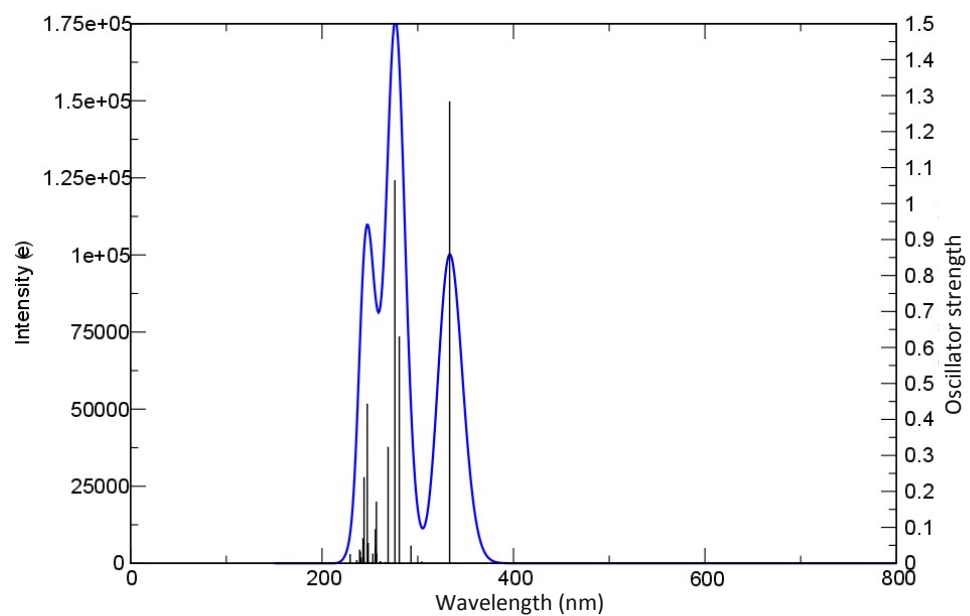
**(P<sub>2</sub>)-DEAbp-UV**



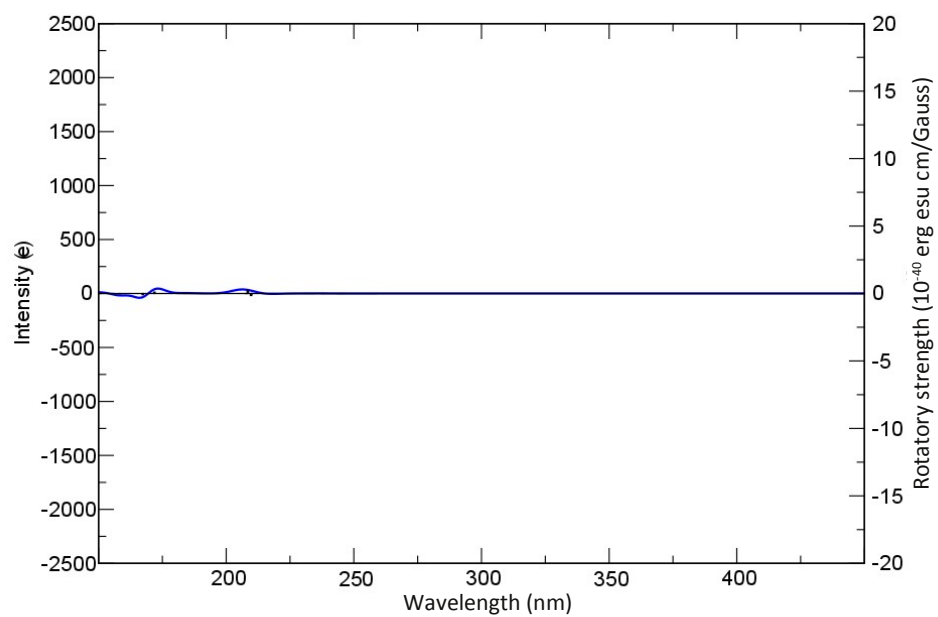
**(P<sub>2</sub>)-DESbp-ECD**



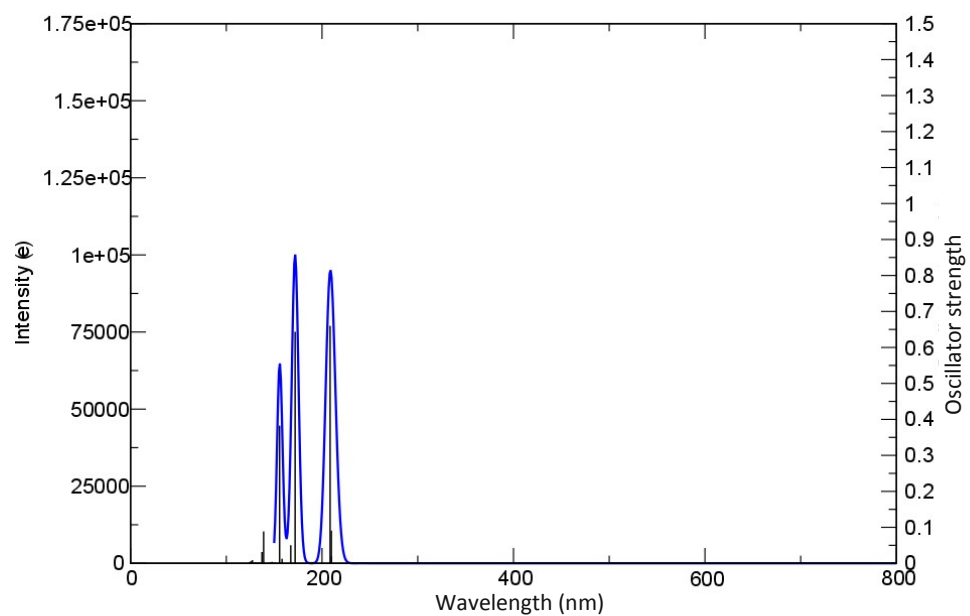
**(P<sub>2</sub>)-DESbp-UV**



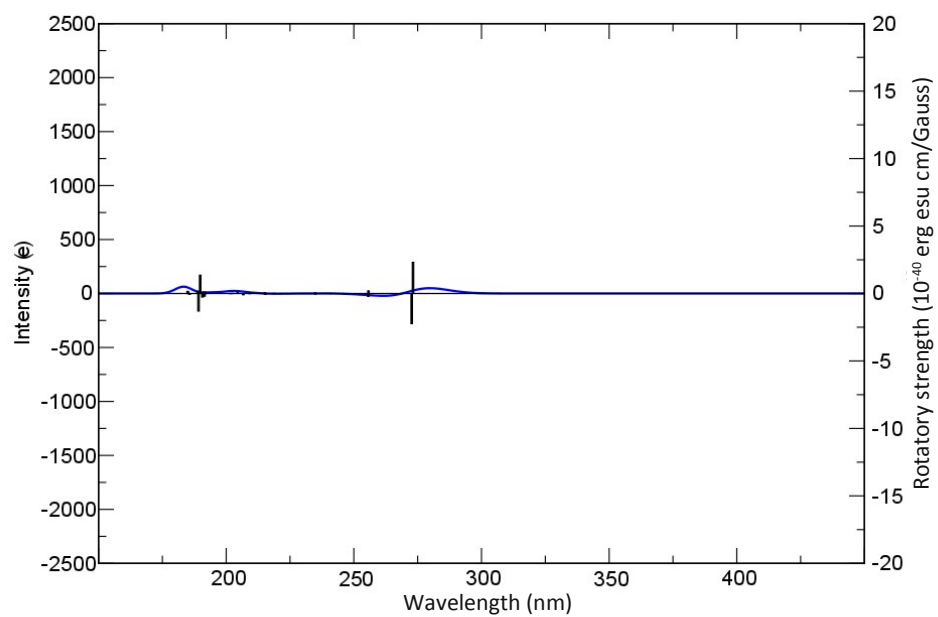
**(P)-DEA-ECD**



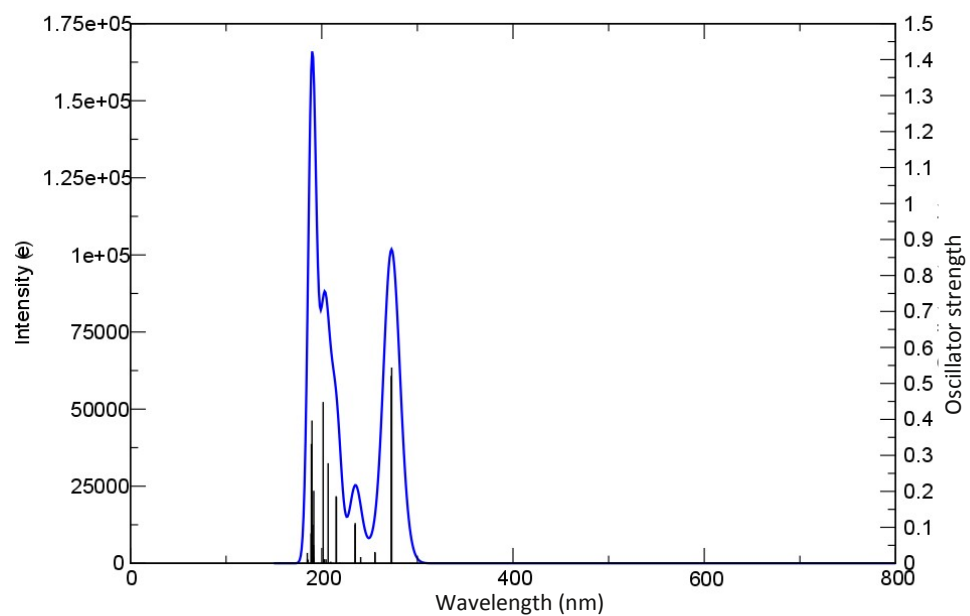
**(P)-DEA-UV**



**(P)-DES-ECD**

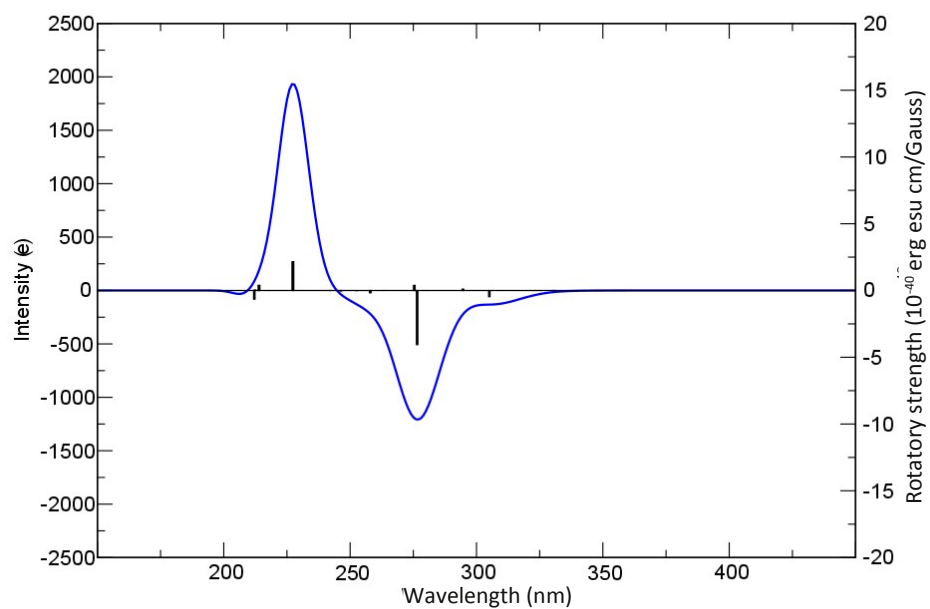


**(P)-DES-UV**

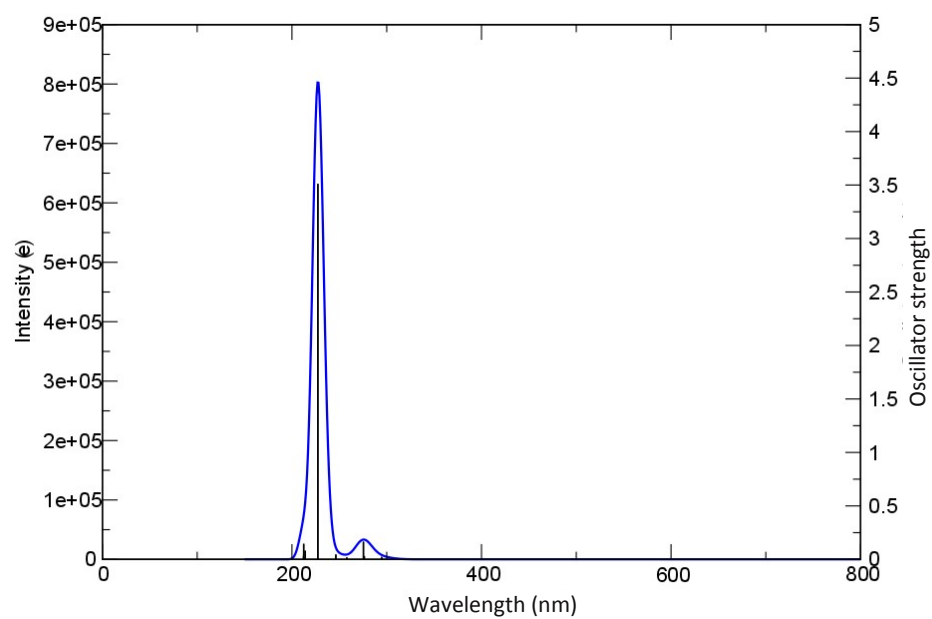


## M062X ECD and UV

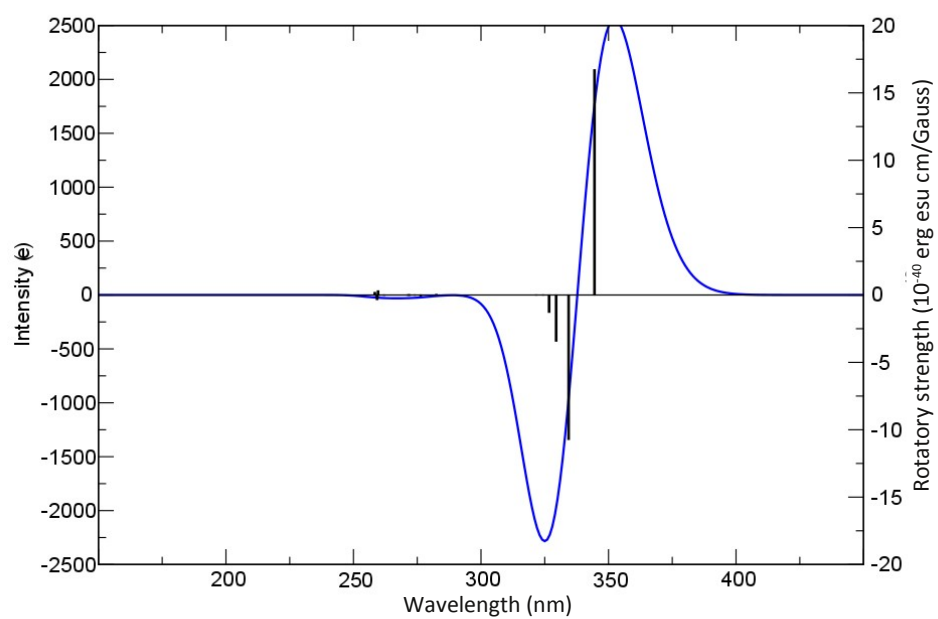
### $(P_4)$ -DEA-ECD



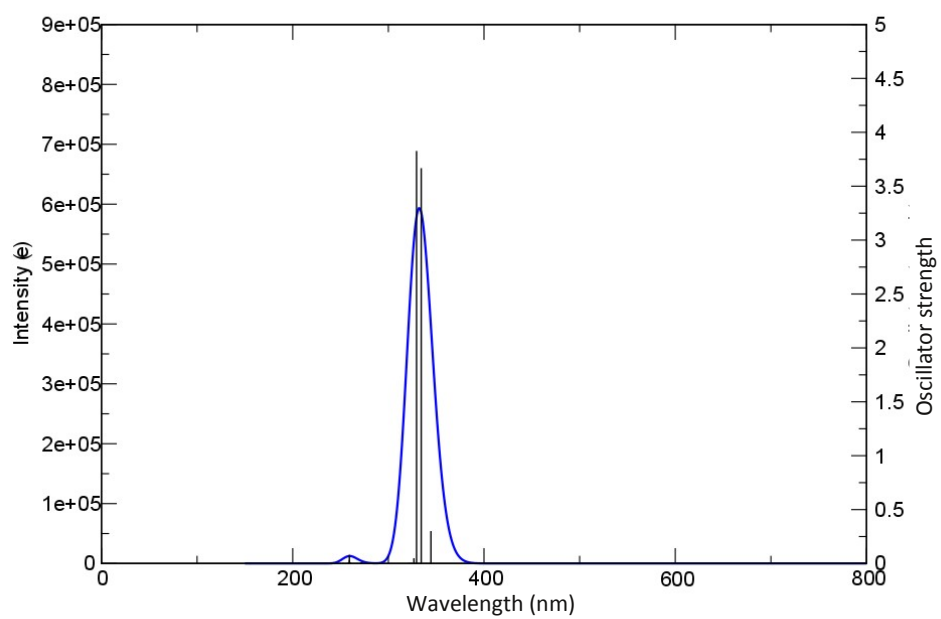
### $(P_4)$ -DEA-UV



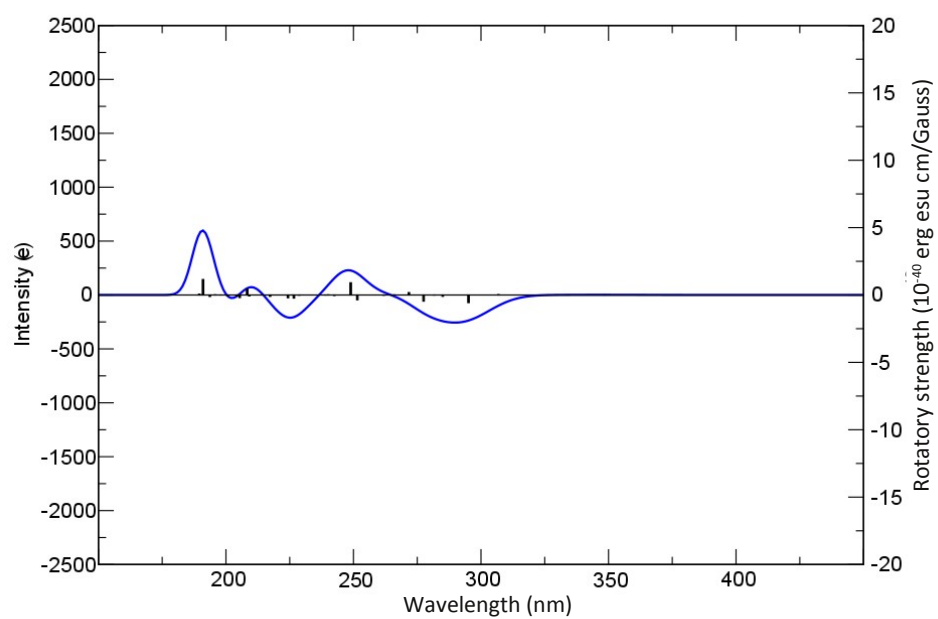
**$(P_4)$ -DES-ECD**



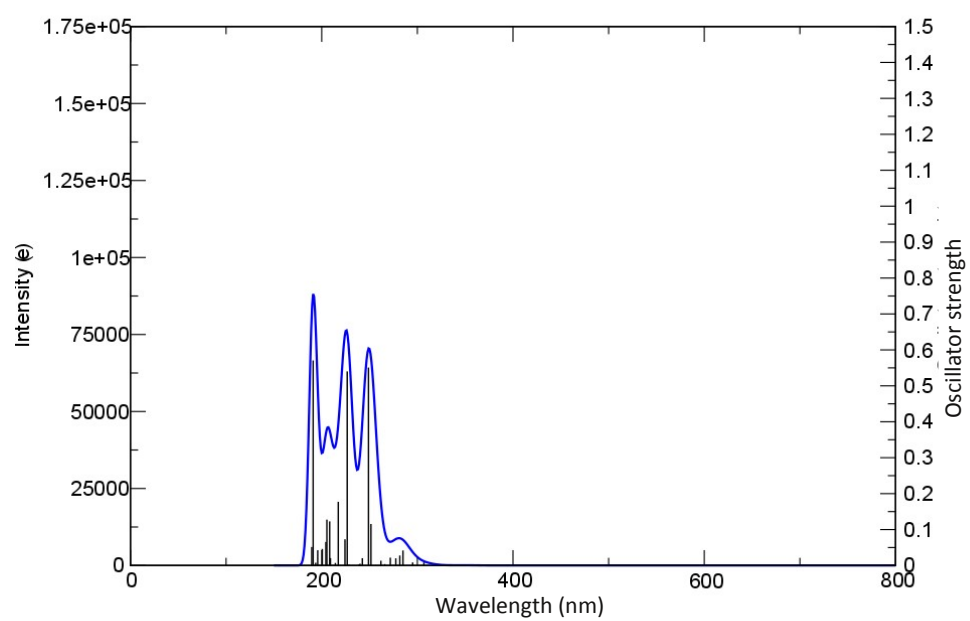
**$(P_4)$ -DES-UV**



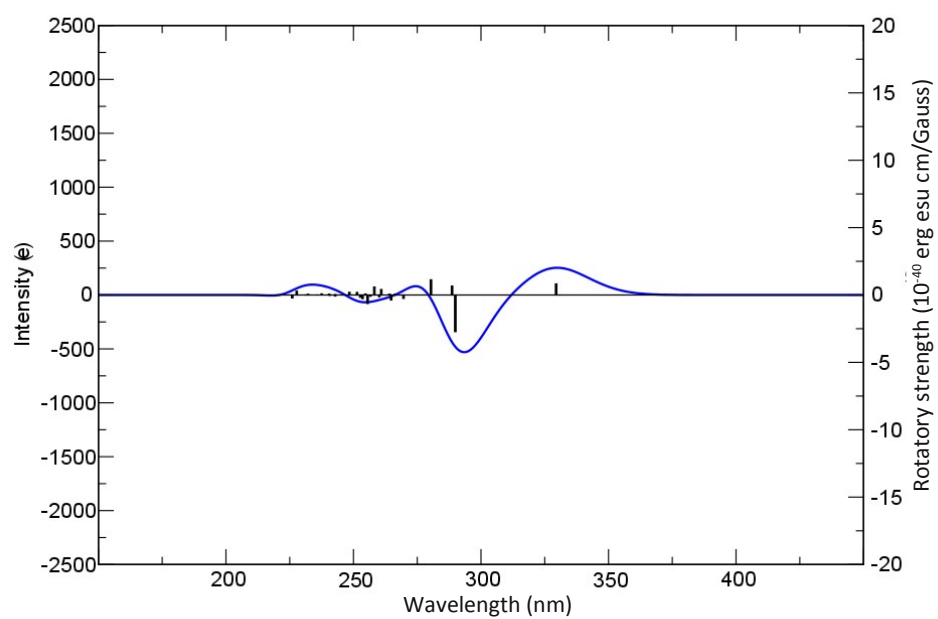
**(P<sub>2</sub>)-DEAp-ECD**



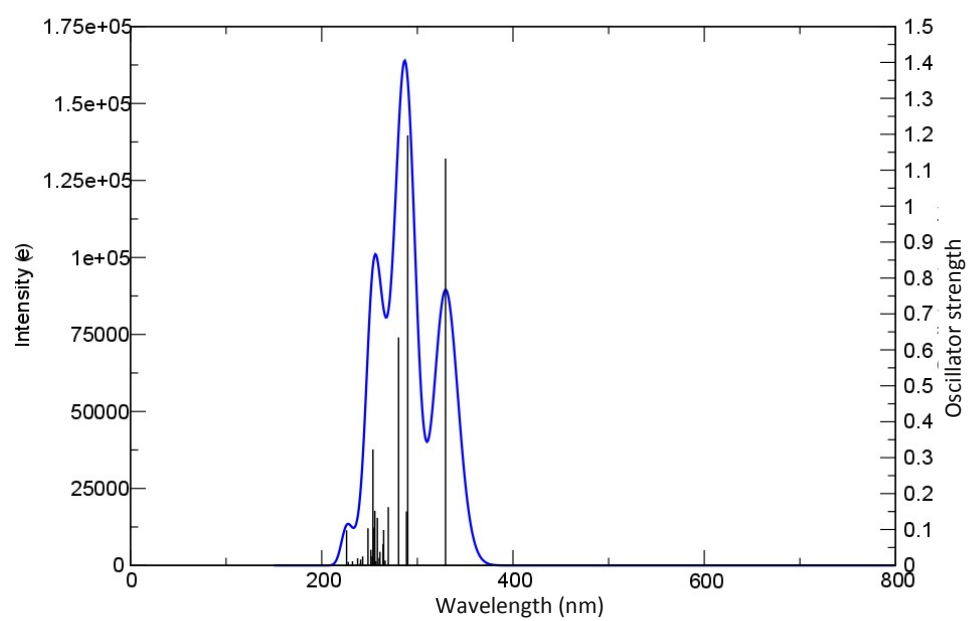
**(P<sub>2</sub>)-DEAp-UV**



**(P<sub>2</sub>)-DESp-ECD**

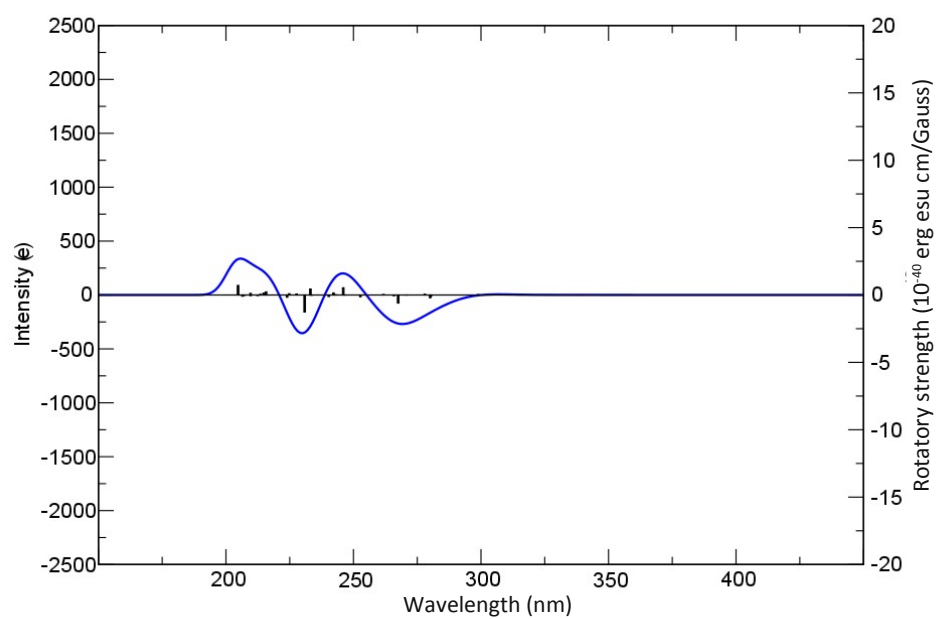


**(P<sub>2</sub>)-DESp-UV**

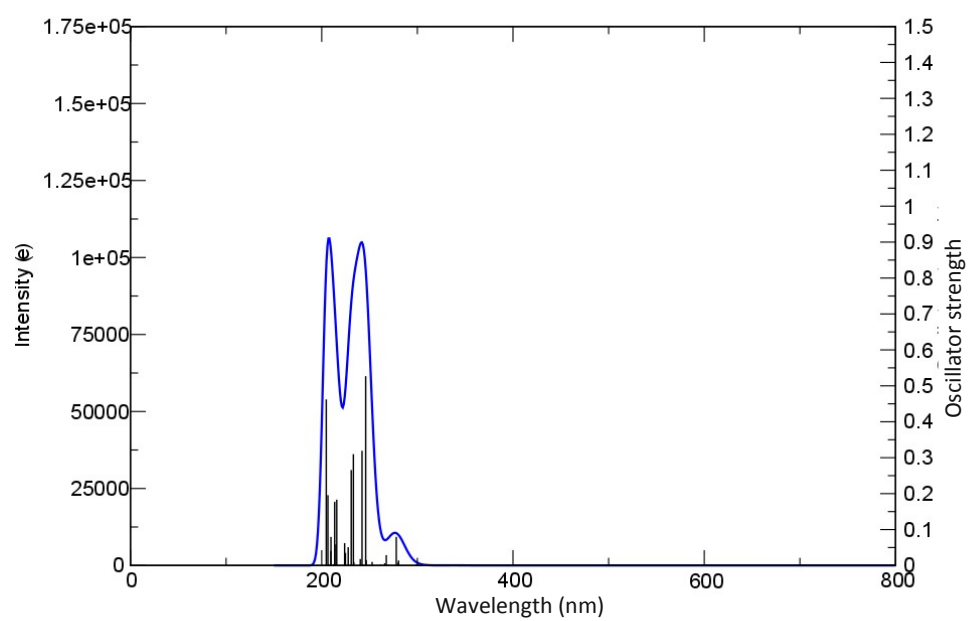




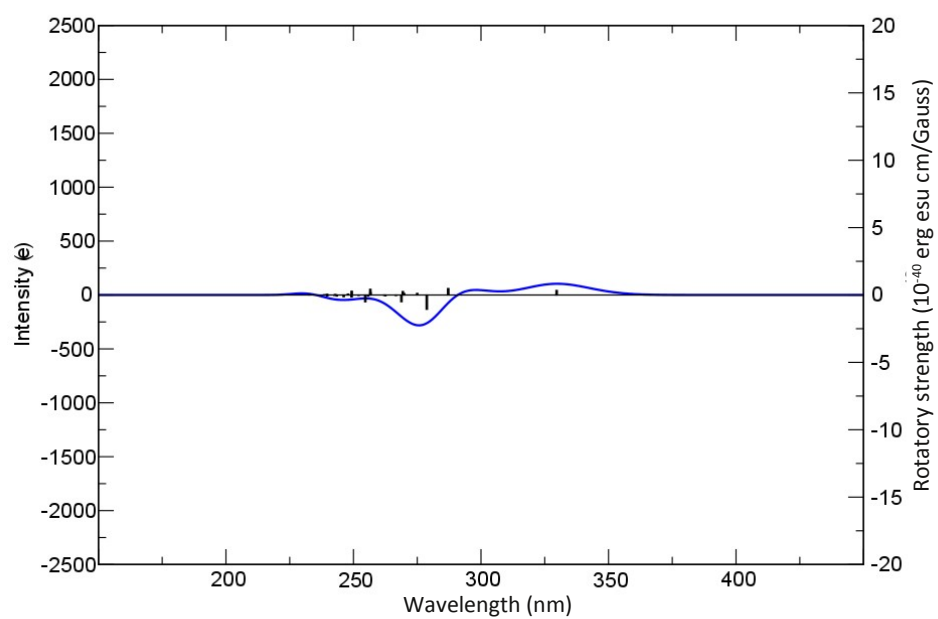
**(P<sub>2</sub>)-DEAbp-ECD**



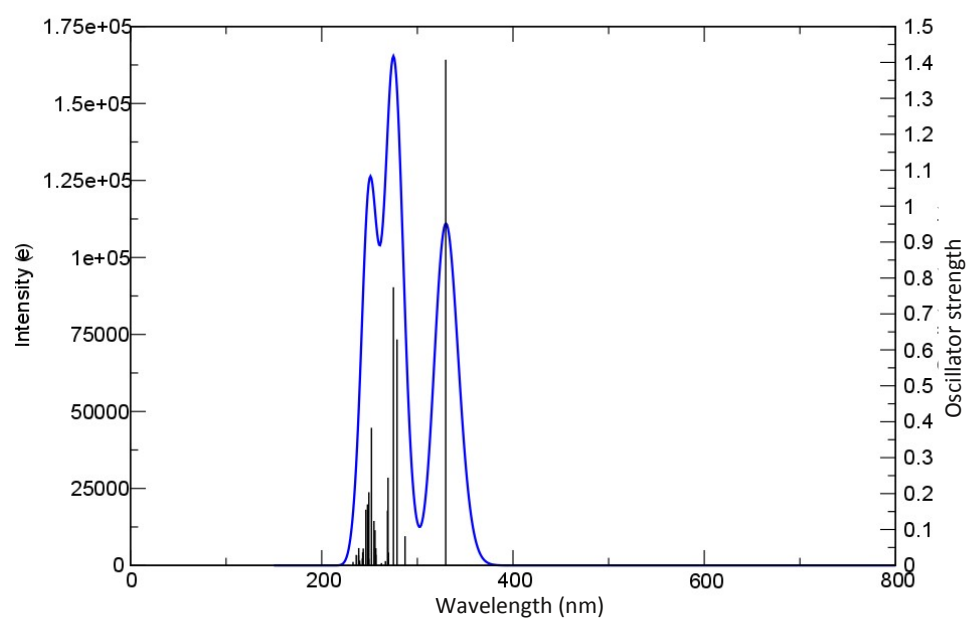
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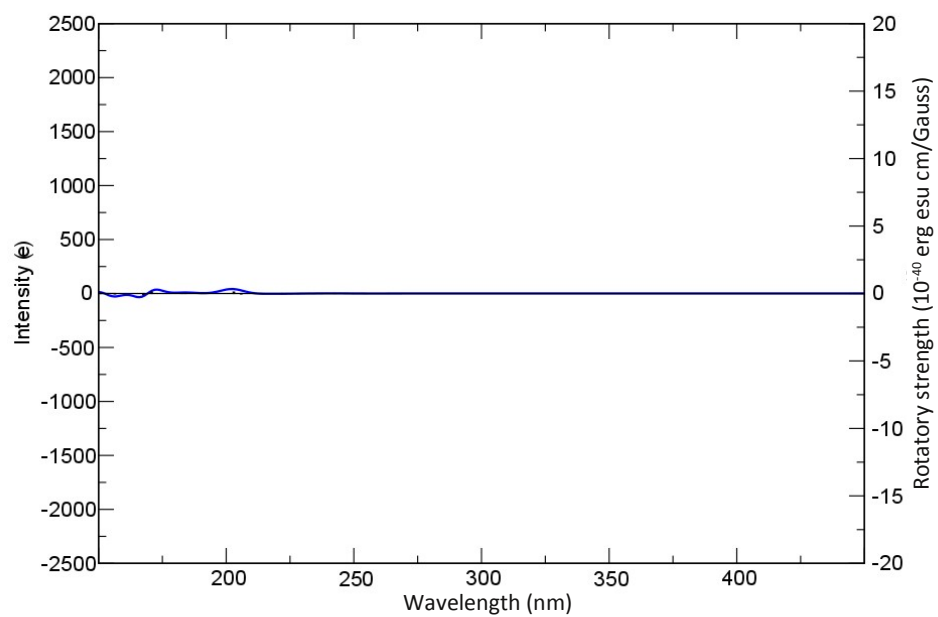
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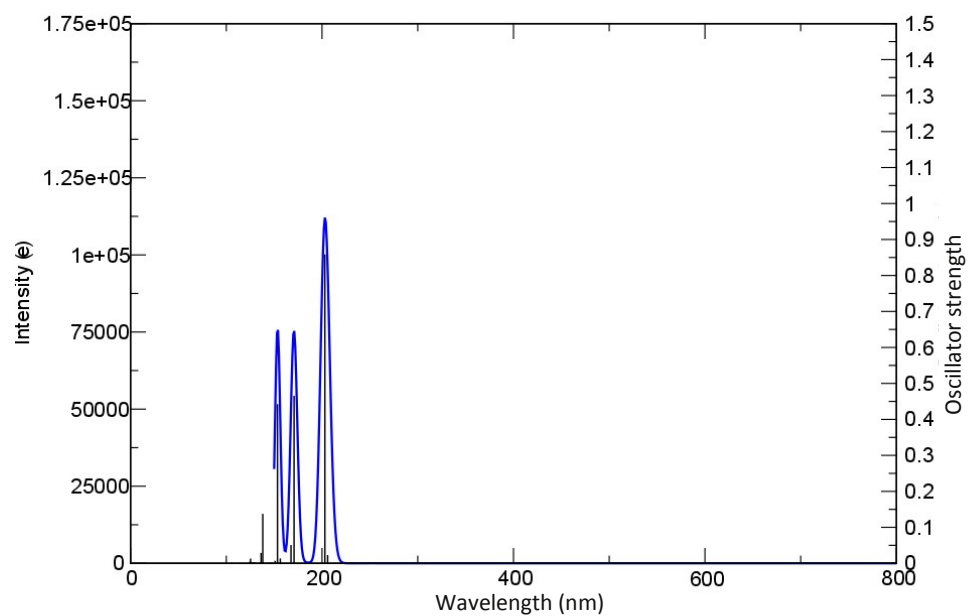
**(P<sub>2</sub>)-DESbp-UV**



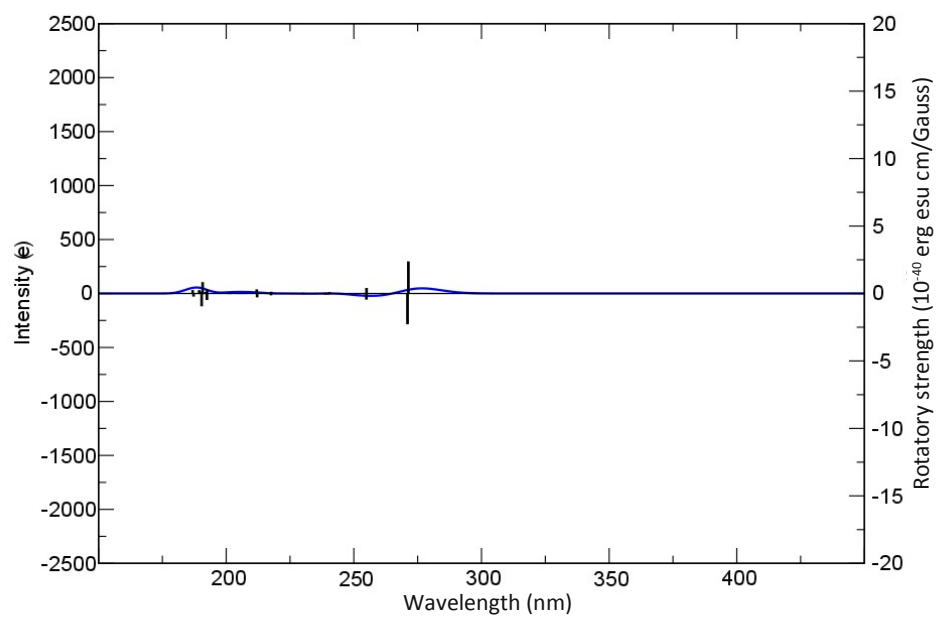
**(P)-DEA-ECD**



**(P)-DEA-UV**



**(P)-DES-ECD**



**(P)-DES-UV**

