Supplementary Material (ESI) for New Journal of Chemistry

Atomic coordinates (in Å), as calculated by DFT, for the 6 derivatives investigated in the manuscript:

"Synthesis and non linear optical characterization of novel boronate derivatives of cinnamaldehyde"
By **Mario Rodríguez** *et al.*

Compound 1a

O	6.87825	3.47661	-7.85947
H	6.61783	4.42255	-7.79998
N	7.96945	5.79184	-7.29078
C	8.89782	2.27288	-7.52222
C	8.82482	4.69749	-7.22413
C	7.72255	9.37213	-6.88424
C	6.85286	10.53848	-6.94500
C	10.18995	4.68282	-6.89209
C	8.18286	3.47245	-7.54083
C	8.33097	7.00420	-7.04415
C	7.38505	8.08551	-7.13467
C	7.39520	11.80357	-6.64733
C	10.24606	2.28860	-7.19034
H	10.80223	1.35485	-7.17596
C	10.89618	3.48943	-6.87483
C	5.48776	10.46558	-7.28858
C	6.61867	12.95217	-6.68761
C	5.27560	12.83674	-7.03136
C	4.69983	11.60340	-7.33307
H	6.37425	7.80192	-7.41911
H	8.38165	1.35027	-7.76872
H	5.03587	9.50721	-7.52411
H	9.35768	7.26815	-6.75838
H	11.95132	3.48665	-6.61707
H	8.75605	9.57927	-6.60423
H	8.44618	11.88069	-6.38007
H	10.70026	5.61053	-6.64640
H	7.03046	13.92838	-6.45955
H	3.64945	11.55716	-7.59617
N	4.44562	14.04065	-7.07751
O	3.26622	13.90575	-7.38384
O	4.98050	15.11012	-6.80707

Compound 2a

O	-3.71621	0.47064	0.59721
N	-1.99892	-1.04025	-0.12601
C	-5.56789	-1.06185	0.32726
C	-3.25964	-1.64025	-0.18258

C	1.53962	-1.79225	-0.49542
C	2.90951	-1.31829	-0.39490
C	-3.62708	-2.93436	-0.56230
C	-1.39497	0.94513	1.57198
C	-4.21534	-0.70040	0.26026
C	-0.87723	-1.66999	-0.35219
C	-0.44478	1.97794	1.56831
C	0.41408	-1.07459	-0.24619
C	-1.59398	0.26372	2.78420
C	3.94991	-2.15869	-0.83725
C	-5.92384	-2.34846	-0.05080
H	-6.96930	-2.64285	-0.00692
C	-1.43172	1.07484	-2.24513
C	-2.04690	1.46468	-1.04903
C	0.28165	2.30989	2.71408
C	-4.96881	-3.28151	-0.49462
C	-2.55205	2.77643	-0.98960
B	-2.24350	0.53423	0.25974
C	-0.87482	0.58516	3.93319
C	3.24704	-0.05530	0.13405
C	5.27633	-1.75957	-0.77364
C	0.07045	1.61086	3.90055
C	5.56793	-0.50252	-0.25342
C	4.56811	0.35433	0.20444
C	-1.80774	3.24433	-3.23929
C	-1.30737	1.94851	-3.32771
C	-2.43502	3.65594	-2.06268
H	0.45950	-0.03336	0.05343
H	-6.30140	-0.33804	0.66688
H	2.47219	0.60530	0.51060
H	-0.93253	-2.72425	-0.62407
H	-2.33543	-0.53226	2.83391
H	-0.27922	2.54274	0.65283
H	-5.28381	-4.27763	-0.79011
H	1.00496	3.12213	2.68157
H	0.63205	1.86682	4.79599
H	1.42740	-2.83006	-0.81207
H	3.70709	-3.13823	-1.24157
H	-2.89300	-3.65563	-0.91141
H	-1.04269	0.06414	-2.35489
H	6.08283	-2.39773	-1.11532
H	-1.05356	0.03956	4.85726
H	4.84100	1.32113	0.61105
H	-2.83548	4.66429	-1.98296
H	-3.04986	3.11090	-0.08174
H	-1.71525	3.92755	-4.08029
H	-0.82463	1.61137	-4.24254
N	6.96522	-0.07039	-0.17901
O	7.19102	1.04140	0.28427
O	7.82143	-0.84765	-0.58556

Compound 1b

N	11.05646	1.13219	-7.12823
O	12.26674	1.23547	-6.95792
O	10.45841	0.06944	-7.24999
O	6.83385	3.40585	-7.64057
H	6.56055	4.34965	-7.67271
N	7.91260	5.78104	-7.38694
C	8.89993	2.27174	-7.38742
C	8.79655	4.71067	-7.29310
C	7.63476	9.33886	-6.83199
C	6.80803	10.53404	-6.91789
C	10.18741	4.75541	-7.11154
C	8.16076	3.44972	-7.44580
C	8.23305	6.98473	-7.05039
C	7.30623	8.07402	-7.18767
C	7.34490	11.75784	-6.48034
C	10.27132	2.36799	-7.18871
C	10.93382	3.58845	-7.05483
C	5.49307	10.52684	-7.42015
C	6.60079	12.93103	-6.53959
C	5.30019	12.90538	-7.03993
H	4.71524	13.81994	-7.08858
C	4.75087	11.69838	-7.47947
H	6.32994	7.82357	-7.59545
H	8.41991	1.30739	-7.49769
H	5.04948	9.59814	-7.76750
H	9.22116	7.23050	-6.63767
H	12.00816	3.60206	-6.91933
H	8.63657	9.50112	-6.43058
H	8.36004	11.78112	-6.08967
H	10.69605	5.71197	-7.03302
H	7.03591	13.86553	-6.19564
H	3.73726	11.67355	-7.87075

Compound 2b

N	11.03825	1.09383	-7.31764
O	12.25505	1.17674	-7.19322
O	10.41818	0.04399	-7.42884
O	6.87580	3.58672	-7.60993
N	7.92561	5.72813	-7.36815
C	8.89086	2.26591	-7.48101
C	8.87095	4.69451	-7.35488
C	7.66416	9.30374	-6.77750
C	6.82784	10.48370	-6.66668
C	10.25777	4.74328	-7.21046
C	5.34929	5.41889	-6.67011
C	8.18088	3.47005	-7.49411

C	8.21249	6.97567	-7.10667
C	4.14488	6.04579	-7.02400
C	7.26465	8.03536	-7.06325
C	5.53426	5.10877	-5.31235
C	7.44626	11.73169	-6.46401
C	10.26858	2.34591	-7.33261
C	6.68274	6.36737	-10.08259
C	6.13151	5.34203	-9.30382
C	3.17366	6.35843	-6.07034
C	10.96801	3.55071	-7.20108
C	5.19133	4.50224	-9.92833
B	6.48463	5.04451	-7.75429
C	4.57328	5.41641	-4.35201
C	5.42188	10.43701	-6.74851
C	6.69307	12.89462	-6.35756
C	3.38716	6.04677	-4.72938
C	5.30300	12.83188	-6.44668
H	4.71007	13.73867	-6.36212
C	4.67252	11.59976	-6.63976
C	5.37152	5.72141	-12.00580
C	6.31049	6.56185	-11.41442
C	4.81271	4.68598	-11.25576
H	6.22449	7.79139	-7.24907
H	8.39128	1.31106	-7.58367
H	4.91449	9.48611	-6.88266
H	9.25358	7.21963	-6.89190
H	6.44717	4.60486	-4.99831
H	3.95787	6.28159	-8.06974
H	12.04555	3.53050	-7.09924
H	2.24587	6.83664	-6.37771
H	2.63298	6.28583	-3.98314
H	8.72990	9.47454	-6.61483
H	8.53086	11.78114	-6.39455
H	10.79033	5.68518	-7.11648
H	7.42907	7.03540	-9.65635
H	7.18878	13.84924	-6.20397
H	4.74522	5.16040	-3.30874
H	3.58896	11.54809	-6.70176
H	4.08272	4.01827	-11.70822
H	4.75201	3.68504	-9.36006
H	5.08045	5.86685	-13.04348
H	6.76107	7.36740	-11.99036

Compound 1c

N	11.11671	1.16780	-7.10341
O	12.33531	1.29703	-7.03216
O	10.53341	0.08911	-7.12313
O	6.82259	3.34778	-7.41287
H	6.53900	4.28804	-7.47465

N	7.86976	5.74295	-7.36369
C	8.92399	2.25645	-7.25773
C	8.77943	4.69581	-7.27930
C	7.59082	9.32066	-6.90180
C	6.77111	10.50689	-6.98188
C	10.17886	4.77122	-7.20680
C	8.16080	3.41680	-7.32017
C	8.18728	6.96487	-7.08136
C	7.25192	8.03995	-7.20844
C	7.31306	11.75099	-6.60707
C	10.30621	2.38353	-7.16743
C	10.95063	3.62019	-7.14663
C	5.43211	10.50777	-7.42251
C	6.58172	12.92303	-6.66194
C	5.23789	12.91677	-7.10475
C	4.68555	11.66722	-7.48492
H	6.25937	7.77668	-7.56609
H	8.45627	1.28016	-7.28232
H	4.96292	9.57577	-7.72567
H	9.19098	7.23049	-6.72043
H	12.03168	3.65864	-7.09415
H	8.61023	9.49054	-6.54932
H	8.34433	11.79412	-6.26202
H	10.67237	5.73890	-7.21860
N	4.49899	14.06999	-7.16467
H	7.05576	13.85035	-6.36116
H	3.66008	11.60778	-7.83156
H	5.95455	15.59217	-7.39604
C	3.13166	14.03576	-7.64072
C	5.09082	15.33066	-6.76855
H	4.34906	16.12414	-6.87098
H	5.42180	15.31202	-5.72104
H	2.72086	15.04636	-7.62487
H	3.06850	13.66248	-8.67225
H	2.49484	13.40317	-7.00695

Compound 2c

N	11.11856	1.20391	-7.03844
O	12.33490	1.31390	-6.92180
O	10.51785	0.13673	-7.07598
O	6.91073	3.59998	-7.48498
N	7.92495	5.76780	-7.39747
C	8.94956	2.32462	-7.27518
C	8.88809	4.75500	-7.31564
C	7.62371	9.37959	-7.04500
C	6.78440	10.54378	-7.00648
C	10.27361	4.83602	-7.18167
C	5.36134	5.46591	-6.65688
C	8.22004	3.51115	-7.36767

C	8.19320	7.03906	-7.22044
C	4.15750	6.08054	-7.03390
C	7.23998	8.08289	-7.25008
C	5.54878	5.21739	-5.28702
C	7.36726	11.81891	-6.85377
C	10.32868	2.43621	-7.13775
C	6.68210	6.16988	-10.15303
C	6.11720	5.22529	-9.28635
C	3.19047	6.43987	-6.09263
C	11.00560	3.65843	-7.09266
C	5.14934	4.36162	-9.83084
B	6.49687	5.03966	-7.72473
C	4.59236	5.57194	-4.33819
C	5.37603	10.49421	-7.10677
C	6.61237	12.97393	-6.81434
C	3.40692	6.18859	-4.73953
C	5.20065	12.91871	-6.92344
C	4.60693	11.63684	-7.06654
C	5.33270	5.40067	-12.00366
C	6.29820	6.26351	-11.49255
C	4.75884	4.44438	-11.16502
H	6.20255	7.81820	-7.42106
H	8.46593	1.35676	-7.30958
H	4.87350	9.53596	-7.20279
H	9.23155	7.30779	-7.02128
H	6.46123	4.72483	-4.95459
H	3.96789	6.27013	-8.08869
H	12.08361	3.66502	-6.99376
H	2.26289	6.90653	-6.41860
H	2.65565	6.46333	-4.00245
H	8.68846	9.56882	-6.89323
H	8.44925	11.89728	-6.76779
H	10.79010	5.79116	-7.15523
N	4.43795	14.05321	-6.88884
H	7.44853	6.85180	-9.78927
H	7.11656	13.92626	-6.69791
H	4.76720	5.36273	-3.28489
H	3.52994	11.54075	-7.14067
H	4.00822	3.75933	-11.55367
H	4.69786	3.60471	-9.19260
H	5.03280	5.46735	-13.04701
H	6.76062	7.00802	-12.13745
H	5.76102	15.56883	-7.54753
C	2.99480	13.96726	-7.00030
C	5.06768	15.34814	-6.72468
H	4.29963	16.12259	-6.71628
H	5.62306	15.41258	-5.77911
H	2.57242	14.97242	-6.96716
H	2.68915	13.50398	-7.94780
H	2.55604	13.38854	-6.17614