Supplementary material

Table 1. CHLA Cartesian coordinates.

Atom	X	Y	Z
Mg	-1.337762	0.130805	0.025296
N01	-2.132623	1.981596	0.222357
N02	-3.192730	-0.684805	-0.374306
N03	-0.586928	-1.727303	-0.158513
N04	0.627654	0.886148	0.410663
O01	3.124581	-4.543803	-0.244677
O02	4.840149	-1.522846	1.708214
O03	3.139917	-2.788308	2.464918
O04	6.067976	1.113986	-2.444252
O05	6.294520	3.330318	-2.125925
C01	-1.463802	3.125076	0.524083
C02	-2.382971	4.241667	0.578149
C03	-3.632879	3.732736	0.291584
C04	-3.460141	2.303528	0.079625
C05	-4.468086	1.400875	-0.230230
C06	-4.358495	0.012689	-0.437091
C07	-5.457786	-0.874333	-0.742893
C08	-4.919597	-2.134070	-0.864166
C09	-3.497567	-1.998664	-0.630098
C10	-2.565783	-3.043461	-0.670209
C11	-1.190583	-2.940377	-0.455949
C12	-0.199064	-3.991688	-0.515314
C13	1.005749	-3.357733	-0.244890
$C13^1$	2.445459	-3.544846	-0.120997
$C13^2$	3.044189	-2.123931	0.199720
C14	0.713531	-1.986792	-0.038253
C15	1.842966	-1.181028	0.210927
C16	1.804384	0.182987	0.406829
C17	2.992806	1.101564	0.600438
C18	2.323196	2.409338	1.071444
C19	0.862827	2.183504	0.716759
C20	-0.078984	3.200750	0.759758
C21	-2.018012	5.643322	0.930991
C22	-4.913335	4.418628	0.239377
C23	-5.119916	5.701047	-0.089084
C24	-6.885169	-0.459542	-0.883147
C25	-5.635979	-3.419785	-1.135623
C26	-5.976281	-4.199906	0.139457
C27	-0.435051	-5.433866	-0.807993
C28	3.796384	-2.107663	1.515259
C29	3.771376	-2.808053	3.746114
C30	3.789379	1.263600	-0.704627
C31	5.108822	2.007002	-0.482354
C32	5.880750	2.255753	-1.754619
C33	6.803000	1.257114	-3.660360
C34	2.495671	2.666062	2.571086
H29(C10)	-2.952832	-4.032927	-0.898105
H31(C05)	-5.468048	1.812626	-0.328360
H43(C22)	-5.784441	3.814128	0.491085
H44(C21)	-2.867206	6.159354	1.390431
H45(C21)	-1.719683	6.227943	0.050692
H46(C21)	-1.182365	5.674928	1.637585
H47(C30)	3.170351	1.795299	-1.439611
H48(C30)	4.010508	0.282016	-1.132634
H49(C27)	-0.910181	-5.574274	-1.786393
H50(C27)	-1.093677	-5.893499	-0.060926
H51(C27)	0.511448	-5.978881	-0.807192
H52(C24)	-7.300486	-0.104125	0.068322
H53(C25)	-5.029419	-4.051544	-1.796915
H54(C25)	-6.559844	-3.213917	-1.689110
H55(C23)	-4.315030	6.359916	-0.398776
H56(C23)	-6.120380	6.122677	-0.083360
H57(C26)	-6.625569	-3.610499	0.794846
H58(C26)	-5.070942	-4.442812	0.705352
H59(C26)	-6.491601	-5.136621	-0.099218
H60(C31)	5.738680	1.409536	0.189666
H61(C31)	4.952115	2.983216	-0.015531
H62(C17)	3.670104	0.700050	1.363480
H63(C18)	2.714406	3.273429	0.519988
H64(C34)	3.554002	2.801613	2.819254
H65(C34)	2.115351	1.820944	3.155574
H66(C34)	1.952872	3.562792	2.886674
H68(C20)	0.309190	4.185006	1.004988
H69($C13^2$)	3.778133	-1.875755	-0.574321
H73(C29)	4.766584	-3.252763	3.674024
H74(C29)	3.863077	-1.794331	4.144407
H75(C29)	3.125410	-3.412939	4.381566
H78(C33)	7.804690	1.645434	-3.459903
H79(C33)	6.859018	0.257186	-4.090054
H80(C33)	6.290508	1.940840	-4.341705
H81(C24)	-7.001433	0.353915	-1.609340
H82(C24)	-7.510953	-1.290875	-1.219900

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Table 2. CHLB Cartesian coordinates.

Atom	X	Y	Z
Mg	-1.185183	0.190978	0.058016
N01	-1.920071	2.062628	0.258255
N02	-3.076964	-0.570088	-0.319087
N03	-1.490386	-0.687733	0.124630
N04	0.805596	0.891304	0.416001
O01	-7.665206	-1.060693	-0.977631
O02	3.136504	-4.612086	-0.232136
O03	3.229325	-2.854507	2.465787
O04	4.947616	-1.620041	1.697592
O05	6.520419	3.145848	-2.200691
O06	6.210449	0.937536	-2.505881
C01	-1.216276	3.186854	0.546113
C02	-2.103911	4.331883	0.609265
C03	-3.369502	3.859147	0.342287
C04	-3.240713	2.422048	0.132276
C05	-4.279198	1.555616	-0.159958
C06	-4.217760	0.158122	-0.367707
C07	-5.338042	-0.709705	-0.651552
C08	-4.829084	-1.997512	-0.782105
C09	-3.415188	-1.884926	-0.567869
C10	-2.505814	-2.955286	-0.608337
C11	-1.131929	-2.887078	-0.407147
C12	-0.168724	-3.967990	-0.468345
C13	1.053251	-3.365555	-0.215482
$C13^1$	2.489932	-3.593119	-0.105687
$C13^2$	3.131629	-2.189141	0.201355
C14	0.801725	-1.984054	-0.015820
C15	1.958799	-1.210953	0.216517
C16	1.962585	0.153893	0.402964
C17	3.179080	1.038110	0.576682
C18	2.553786	2.368146	1.045316
C19	1.083454	2.181654	0.712115
C20	0.171947	3.226839	0.762716
C21	-1.691540	5.722358	0.952706
C22	-4.630750	4.581718	0.306543
C23	-4.802440	5.860993	-0.051334
C24	-6.724862	-0.302298	-0.797261
C25	-5.594677	-3.250119	-1.056700
C26	-6.229302	-3.838708	0.209069
C27	-0.448518	-5.404355	-0.747620
C28	3.892649	-2.186617	1.512767
C29	3.867683	-2.887332	3.744104
C30	3.965206	1.166866	-0.738613
C31	5.307651	1.873687	-0.537308
C32	6.072797	2.088401	-1.820252
C34	2.753930	2.633235	2.540233
H29(C10)	-2.922459	-3.935159	-0.822595
H31(C05)	-5.262547	2.006014	-0.243095
H43(C22)	-5.513282	4.012418	0.597027
H44(C21)	-2.526734	6.273909	1.395655
H45(C21)	-1.360408	6.285165	0.070117
H46(C21)	-0.864082	5.729815	1.669629
H47(C30)	3.353382	1.710040	-1.471225
H48(C30)	4.153224	0.176001	-1.160902
H49(C27)	-0.938678	-5.536963	-1.719492
H50(C27)	-1.112067	-5.838289	0.010156
H51(C27)	0.481805	-5.976258	-0.753066
H52(C24)	-6.912538	0.791536	-0.740441
H53(C25)	-4.938411	-3.994706	-1.522546
H54(C25)	-6.392239	-3.024606	-1.770491
H55(C23)	-3.983609	6.482412	-0.399846
H56(C23)	-5.787478	6.316896	-0.032333
H57(C26)	-6.948387	-3.132014	0.631142
H58(C26)	-5.472066	-4.061728	0.968140
H59(C26)	-6.762177	-4.765569	-0.027316
H60(C31)	5.927739	1.264815	0.133569
H61(C31)	5.184870	2.858388	-0.078183
H62(C17)	3.852219	0.621182	1.334964
H63(C18)	2.960881	3.216149	0.480672
H64(C34)	3.819074	2.740512	2.771774
H65(C34)	2.358229	1.804716	3.138029
H66(C34)	2.242080	3.548163	2.855039
H68(C20)	0.590445	4.200843	0.997918
H69($C13^2$)	3.866646	-1.966758	-0.579350
H73(C29)	4.853731	-3.350699	3.665512
H74(C29)	3.980321	-1.875764	4.142253
H75(C29)	3.213911	-3.480607	4.382337
H78(C33)	6.937346	1.047836	-3.730775
H79(C33)	7.954654	1.399760	-3.542511
H80(C33)	6.951806	0.044560	-4.155930
H81(C24)	6.442957	1.746903	-4.409833

Table 3. BCRY Cartesian coordinates.

Atom	X	Y	Z
O01	-14.746335	-2.254986	-0.577559

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C01	-12.296896	0.660895	-0.680431	H46(C02)	-12.913816	-0.949280	-1.998138
C01’	13.100445	-0.549387	0.709982	H47(C08)	-8.531224	-0.671439	-0.021093
C02	-13.337423	-0.355472	-1.176910	H48(C10)	-6.309997	-0.447652	0.001824
C02’	14.141624	0.460774	1.218524	H49(C19)	-8.297039	3.161739	0.117258
C03	-13.789275	-1.321596	-0.097927	H50(C19)	-6.787638	3.135031	1.033197
C03’	14.602990	1.423526	0.137984	H51(C19)	-8.307586	2.683107	1.813059
C04	-12.597195	-2.118715	0.387482	H52(C11)	-4.978815	2.251091	0.735047
C04’	13.415156	2.226205	-0.372638	H53(C12)	-3.939435	-0.521310	-0.064209
C05	-11.367563	-1.285855	0.655056	H54(C14)	-1.724538	-0.803604	-0.185427
C05’	12.176358	1.401279	-0.627441	H55(C20)	-2.864354	3.158887	0.038660
C06	-11.205626	-0.038923	0.147740	H56(C20)	-2.836365	2.679483	1.735109
C06’	12.011290	0.155501	-0.117847	H57(C20)	-1.326671	2.794469	0.826549
C07	-10.005408	0.773098	0.375249	H58(C15)	0.218753	1.528085	0.437266
C07’	10.807230	-0.651625	-0.343469	H59(C15’)	0.582734	-1.395688	-0.395887
C08	-8.721284	0.360816	0.269782	H60(C14’)	2.526950	0.935361	0.226207
C08’	9.524073	-0.236896	-0.235771	H61(C12’)	4.742175	0.651671	0.103699
C09	-7.544317	1.178164	0.478172	H62(C20’)	3.664684	-3.027675	0.002111
C09’	8.345291	-1.052262	-0.442203	H63(C20’)	3.635762	-2.548587	-1.694373
C10	-6.318267	0.603039	0.295841	H64(C20’)	2.126625	-2.662711	-0.784763
C10’	7.120258	-0.475285	-0.258490	H65(C11’)	5.778532	-2.121686	-0.695968
C11	-5.030293	1.205404	0.442075	H66(C10’)	7.113822	0.575481	0.035294
C11’	5.831378	-1.075993	-0.403203	H67(C08’)	9.336049	0.795575	0.055619
C12	-3.867908	0.526657	0.230179	H68(C19’)	9.095873	-3.036538	-0.081983
C12’	4.669705	-0.396283	-0.190470	H69(C19’)	7.584535	-3.008415	-0.994807
C13	-2.537468	1.055158	0.355101	H70(C19’)	9.103574	-2.558845	-1.777929
C13’	3.338797	-0.923908	-0.314465	H71(C07’)	10.981867	-1.706476	-0.556809
C14	-1.479392	0.220589	0.099564	H72(C04’)	13.162694	3.018064	0.352128
C14’	2.281238	-0.088741	-0.058579	H73(C04’)	13.684472	2.759640	-1.294477
C15	-0.089441	0.521655	0.158639	H74(C02’)	13.698523	1.039508	2.041705
C15’	0.891186	-0.389310	-0.117300	H75(C02’)	14.990783	-0.089180	1.645428
C16	-11.681932	1.333403	-1.918060	H76(C03’)	15.378774	2.095720	0.523381
C16’	12.479805	-1.230162	1.940141	H77(C03’)	15.057086	0.868587	-0.692568
C17	-12.984509	1.742983	0.173279	H78(C18)	-9.834789	-2.771728	0.999399
C17’	13.791023	-1.623836	-0.149235	H79(C18)	-9.618472	-1.291718	1.944184
C18	-10.366588	-1.975713	1.539627	H80(C18)	-10.880230	-2.465696	2.376413
C18’	11.170302	2.096717	-1.502526	H81(C18’)	11.678834	2.592466	-2.339341
C19	-7.733102	2.612184	0.881489	H82(C18’)	10.639701	2.888755	-0.954994
C19’	8.531012	-2.486763	-0.845304	H83(C18’)	10.420181	1.415536	-1.908311
C20	-2.372920	2.493251	0.758652	H84(C16)	-10.987351	2.134840	-1.647285
C20’	3.173056	-2.361979	-0.717659	H85(C16)	-12.472181	1.770892	-2.540366
H42(C07)	-10.183022	1.827400	0.588545	H86(C16)	-11.131744	0.607712	-2.526580
H43(C04)	-12.871200	-2.681014	1.289032	H87(C17)	-13.742995	2.269787	-0.418955
H44(C04)	-12.370125	-2.879989	-0.375619	H88(C17)	-13.473204	1.316450	1.054781
H45(C02)	-14.199702	0.188722	-1.590641	H89(C17)	-12.268499	2.493374	0.525376

H90(C17')	13.075337	-2.362657	-0.525998
H91(C17')	14.536692	-2.165403	0.445916
H92(C17')	14.296768	-1.185995	-1.015457
H93(C16')	13.268750	-1.667730	2.564181
H94(C16')	11.924655	-0.508991	2.549946
H95(C16')	11.788626	-2.032930	1.664623
H96(C03)	-14.210039	-0.758624	0.751226
H97(O01)	-15.514562	-1.751551	-0.882472

Table 4. ZEA Cartesian coordinates.

Atom	X	Y	Z
O01	-15.231274	-2.130375	0.314398
O02	15.176173	2.227323	0.208276
C01	-12.662823	0.529758	0.969481
C01'	12.663602	-0.534427	0.965400
C02	-13.720715	-0.554665	1.225699
C02'	13.713139	0.558717	1.221847
C03	-14.212525	-1.209059	-0.044780
C03'	14.211993	1.217165	-0.050695
C04	-13.042856	-1.892602	-0.734384
C04'	13.049406	1.884093	-0.754744
C05	-11.804902	-1.033858	-0.836812
C05'	11.809845	1.027884	-0.842253
C06	-11.608355	0.046211	-0.041272
C06'	11.608909	-0.049561	-0.044049
C07	-10.399760	0.875598	-0.097365
C07'	10.398576	-0.876493	-0.096192
C08	-9.121140	0.435643	-0.138011
C08'	9.120326	-0.435433	-0.137189
C09	-7.935777	1.266950	-0.164873
C09'	7.934259	-1.265759	-0.162640
C10	-6.715539	0.651956	-0.168194
C10'	6.714432	-0.649911	-0.166841
C11	-5.421767	1.259379	-0.185668
C11'	5.420286	-1.256546	-0.182985
C12	-4.265601	0.538322	-0.186210
C12'	4.264454	-0.534942	-0.184880
C13	-2.930379	1.069521	-0.197172
C13'	2.929038	-1.065676	-0.194765
C14	-1.879668	0.187874	-0.195072
C14'	1.878552	-0.183748	-0.194535
C15	-0.487002	0.482048	-0.198286
C15'	0.485842	-0.477696	-0.197228
C16	-12.000198	0.851077	2.318698
C16'	12.003303	-0.864703	2.313435
C17	-13.340278	1.808252	0.440993
C17'	13.348907	-1.806348	0.431493
C18	-10.844336	-1.490969	-1.899081
C18'	10.846266	1.487426	-1.900865
C19	-8.110074	2.758240	-0.183815
C19'	8.107203	-2.757266	-0.179288
C20	-2.753067	2.561658	-0.208591
C20'	2.751229	-2.557788	-0.203168
H43(O01)	-15.536007	-2.558502	-0.498339
H44(O02)	15.925949	1.805554	0.651602
H45(C02)	-13.296916	-1.341868	1.863906
H46(C02)	-14.568699	-0.124502	1.772436
H47(C02')	13.282327	1.345468	1.855790
H48(C02')	14.553179	0.123083	1.783420
H49(C03)	-14.624932	-0.439845	-0.718113
H50(C03')	14.641823	0.453577	-0.719431
H51(C04)	-12.811778	-2.811633	-0.172521
H52(C04)	-13.337348	-2.225398	-1.741102
H53(C04')	12.819064	2.815041	-0.212811
H54(C04')	13.357696	2.199228	-1.759580
H55(C07)	-10.563271	1.951319	-0.032317
H56(C07')	10.560420	-1.952570	-0.029668
H57(C17')	14.081002	-2.177972	1.159137
H58(C17')	12.626074	-2.610835	0.258260
H59(C17')	13.868307	-1.622569	-0.514158
H60(C16')	11.298823	-1.698473	2.232349
H61(C16')	11.453647	-0.001234	2.703220
H62(C16')	12.768031	-1.142516	3.049041
H63(C17)	-13.861143	1.631396	-0.505206
H64(C17)	-12.614062	2.610678	0.272152
H65(C17)	-14.071505	2.177805	1.169967
H66(C16)	-12.764105	1.128270	3.055074
H67(C16)	-11.454911	-0.016897	2.704711
H68(C16)	-11.291843	1.681924	2.241346
H69(C18)	-11.391613	-1.750971	-2.814338
H70(C18)	-10.309552	-2.401603	-1.593788
H71(C18)	-10.097279	-0.734450	-2.146056
H72(C18')	10.095692	0.733493	-2.144771
H73(C18')	10.316292	2.399775	-1.592579
H74(C18')	11.391259	1.746308	-2.817399
H75(C08)	-9.121140	0.435643	-0.138011
H76(C08')	8.942102	0.638941	-0.123944
H77(C10)	-6.717575	-0.439028	-0.153722

H78(C10')	6.714432	-0.649911	-0.166841
H79(C19)	-7.160052	3.292926	-0.226377
H80(C19)	-8.643779	3.100553	0.711726
H81(C19)	-8.707807	3.069995	-1.048894
H82(C19')	8.641163	-3.098701	0.716463
H83(C19')	8.704071	-3.070885	-1.044289
H84(C19')	7.156685	-3.291184	-0.220385
H85(C11)	-5.360476	2.344738	-0.196489
H86(C11')	5.358348	-2.341897	-0.191733
H87(C12)	-4.346476	-0.549489	-0.175000
H88(C12')	4.264454	-0.534942	-0.184880
H89(C14)	-2.133832	-0.873082	-0.188350
H90(C14')	2.132958	0.877150	-0.190045
H91(C15)	-0.170095	1.523714	-0.199882
H92(C15')	0.168822	-1.519338	-0.196635
H93(C20)	-3.232766	3.004233	-1.090032
H94(C20)	-3.220719	3.016688	0.672978
H95(C20)	-1.704155	2.861071	-0.218232
H96(C20')	1.702222	-2.856896	-0.211997
H97(C20')	3.230622	-3.002249	-1.083825
H98(C20')	3.218923	-3.011205	0.679212

Table 5. LUT Cartesian coordinates.

Atom	X	Y	Z
O01	-14.266680	2.889849	-0.095269
O02	15.049525	-2.056666	0.385980
C01	-12.286869	-0.022221	1.176362
C01'	12.489386	0.716395	0.904152
C02	-13.459729	0.946593	0.978930
C02'	13.559530	-0.330157	1.252893
C03	-13.059155	2.205908	0.232985
C03'	14.065880	-1.091624	0.042218
C04	-12.282356	1.852701	-1.002678
C04'	12.913288	-1.840323	-0.592768
C05	-11.711302	0.665616	-1.240878
C05'	11.657579	-1.018372	-0.750127
C06	-11.787587	-0.477651	-0.237568
C06'	11.439993	0.123108	-0.051468
C07	-10.536547	-1.318564	-0.151641
C07'	10.214278	0.919593	-0.172818
C08	-9.273459	-0.854956	-0.204054
C08'	8.944907	0.452013	-0.165159
C09	-8.063169	-1.647552	-0.087072
C09'	7.742037	1.251714	-0.267573
C10	-6.860635	-1.006294	-0.159418
C10'	6.535401	0.613333	-0.207542
C11	-5.550838	-1.575115	-0.069806
C11'	5.228573	1.187103	-0.286696
C12	-4.413704	-0.830413	-0.152272
C12'	4.088984	0.443994	-0.212039
C13	-3.065203	-1.323106	-0.074107
C13'	2.741945	0.939678	-0.284539
C14	-2.036698	-0.421909	-0.174881
C14'	1.711918	0.039257	-0.188622
C15	-0.637083	-0.678825	-0.127011
C15'	0.312661	0.297456	-0.235271
C16	-11.175721	0.660919	1.982673
C16'	12.489386	0.716395	0.904152
C17	-12.783792	-1.241441	1.958075
C17'	13.149367	1.946575	0.253299
C18	-11.098857	0.367192	-2.581642
C18'	10.698949	-1.589313	-1.757756
C19	-8.202916	-3.129331	0.108243
C19'	7.884164	2.737343	-0.432924
C20	-2.852096	-2.798567	0.113926
C20'	2.530572	2.416820	-0.461531
H43(O01)	-14.022687	3.723382	-0.522040
H44(O02)	15.793166	-1.583149	0.785189
H46(C02)	-14.250864	0.460026	0.393088
H47(C02)	-13.896517	1.214908	1.948759
H48(C03)	-12.450549	2.849631	0.891783
H49(C17)	-11.982662	-1.973481	2.109175
H50(C17)	-13.609199	-1.741001	1.436281
H51(C17)	-13.148183	-0.941027	2.947432
H52(C16)	-10.697456	1.470024	1.420848
H53(C16)	-10.393943	-0.050435	2.262723
H54(C16)	-11.590434	1.088093	2.903555
H55(C02')	14.393403	0.169368	1.768569
H56(C02')	13.145424	-1.064037	1.957438
H57(C04)	-12.238118	2.622161	-1.775890
H58(C03')	14.478953	-0.383709	-0.694862
H59(C07)	-10.697187	-2.384357	0.000279
H60(C04')	13.223630	-2.238805	-1.566901
H61(C04')	12.702586	-2.722867	0.031836
H62(C17')	13.876697	2.396320	0.940523
H63(C17')	13.669228	1.686690	-0.674055
H64(C17')	12.411218	2.718615	0.010841
H65(C16')	12.589710	1.513327	2.923361

H66(C16')	11.107937	1.966414	2.066677
H67(C16')	11.295016	0.322154	2.689208
H68(C18)	-10.028824	0.147019	-2.520113
H69(C18)	-11.567917	-0.521401	-3.025462
H70(C18)	-11.241440	1.203682	-3.272295
H71(C08)	-9.121215	0.215918	-0.346773
H72(C07')	10.355942	1.999977	-0.209358
H73(C18')	11.245347	-1.918974	-2.650426
H74(C18')	9.932858	-0.874824	-2.064083
H75(C18')	10.188167	-2.480267	-1.365886
H76(C08')	8.788500	-0.619502	-0.048354
H77(C19)	-7.240500	-3.638192	0.179139
H78(C19)	-8.759115	-3.581004	-0.722420
H79(C19)	-8.765317	-3.350305	1.023965
H80(C10)	-6.889694	0.075059	-0.302153
H81(C19')	8.471751	2.975770	-1.327754
H82(C19')	6.922685	3.245315	-0.521252
H83(C19')	8.413857	3.176394	0.421887
H84(C10')	6.561187	-0.470463	-0.084508
H85(C11)	-5.463122	-2.649636	0.069961
H86(C11')	5.143260	2.263635	-0.412133
H87(C12)	-4.521122	0.246244	-0.291211
H88(C12')	4.194451	-0.634264	-0.084771
H89(C14)	-2.316228	0.624163	-0.308552
H90(C14')	1.990313	-1.007799	-0.060570
H91(C15)	-0.295680	-1.704577	0.002343
H92(C15')	-0.028321	1.323477	-0.363860
H93(C20)	-1.796338	-3.069332	0.158268
H94(C20)	-3.306545	-3.365796	-0.707442
H95(C20)	-3.323222	-3.145229	1.041740
H96(C20')	2.984774	2.977122	0.364712
H97(C20')	3.002963	2.770161	-1.386134
H98(C20')	1.475092	2.688991	-0.504436

Table 6. VIO Cartesian coordinates.

Atom	X	Y	Z
O01	-12.679680	4.472756	0.037420
O01'	14.263388	3.310772	-0.049565
O02	-9.507657	1.683256	-0.254520
O02'	10.250347	1.975360	-0.245431
C01	-11.435550	1.124849	1.250225
C01'	11.838811	0.723772	1.238256
C02	-12.350702	2.332184	0.969588
C02'	13.145948	1.476122	0.923004
C03	-11.732770	3.415886	0.110687
C03'	12.981270	2.707007	0.055875
C04	-11.428196	2.846930	-1.268615
C04'	12.450550	2.289034	-1.308801
C05	-10.572646	1.601684	-1.213618
C05'	11.178934	1.476245	-1.219290
C06	-10.568878	0.753580	0.019401
C06'	10.870205	0.707936	0.027601
C07	-10.154180	-0.673288	-0.065639
C07'	9.931051	-0.445174	-0.028502
C08	-8.867439	-1.068203	-0.095613
C08'	8.591382	-0.309717	-0.035487
C09	-8.410157	-2.443203	-0.157892
C09'	7.622480	-1.388306	-0.074219
C10	-7.084729	-2.770977	-0.174205
C10'	6.297408	-1.061962	-0.071017
C11	-5.956160	-1.888875	-0.136691
C11'	5.171500	-1.944213	-0.105409
C12	-4.671825	-2.337944	-0.155444
C12'	3.884780	-1.498686	-0.096499
C13	-3.484832	-1.525672	-0.119336
C13'	2.700151	-2.313064	-0.131032
C14	-2.267199	-2.154566	-0.143312
C14'	1.480932	-1.686527	-0.112980
C15	-0.972750	-1.560936	-0.115782
C15'	0.187272	-2.281579	-0.140491
C16	-10.475300	1.430769	2.408072
C16'	11.098284	1.390538	2.405771
C17	-12.343097	-0.041674	1.664580
C17'	12.228680	-0.700276	1.657695
C18	-10.192051	1.042906	-2.560002
C18'	10.582464	1.097958	-2.550062
C19	-9.442212	-3.534543	-0.200886
C19'	8.131587	-2.799901	-0.113183
C20	-3.641543	-0.032811	-0.056137
C20'	2.859013	-3.806203	-0.184852
H45(O01)	-12.281357	5.184529	-0.483380
H46(O01')	14.162797	4.115785	-0.577158
H47(C04)	-10.912320	3.595338	-1.889255
H48(C04)	-12.379534	2.621039	-1.768231
H49(C04')	12.254043	3.173688	-1.933546
H50(C04')	13.228272	1.705795	-1.819411
H51(C07)	-10.956077	-1.406692	-0.085412

H52(C07')	10.383489	-1.433333	-0.049173
H53(C02)	-12.674923	2.768135	1.922124
H54(C02)	-13.261244	1.994285	0.454876
H55(C02')	13.634693	1.759906	1.862782
H56(C02')	13.841712	0.805178	0.399547
H57(C03)	-10.799041	3.771889	0.569008
H58(C03')	12.269683	3.403047	0.522495
H59(C18)	-9.601456	1.781351	-3.114252
H60(C18)	-9.602684	0.129745	-2.462162
H61(C18)	-11.088808	0.821772	-3.149800
H62(C18')	10.313407	2.003205	-3.106354
H63(C18')	11.309837	0.540352	-3.150929
H64(C18')	9.686773	0.486877	-2.427229
H65(C17)	-13.006266	0.284285	2.473693
H66(C17)	-11.768208	-0.897963	2.031119
H67(C17)	-12.977484	-0.378909	0.836012
H68(C16)	-11.040219	1.628199	3.326181
H69(C16)	-9.850835	2.301138	2.189598
H70(C16)	-9.809735	0.580506	2.594161
H71(C16')	10.857342	2.433247	2.182396
H72(C16')	11.714710	1.360893	3.311455
H73(C16')	10.158182	0.868596	2.616272
H74(C17')	12.983406	-0.651498	2.450657
H75(C17')	11.373088	-1.260822	2.047245
H76(C17')	12.663576	-1.265803	0.824773
H77(C08)	-8.118692	-0.280772	-0.074849
H78(C08')	8.192679	0.703589	-0.015369
H79(C10)	-6.840032	-3.832863	-0.219488
H80(C10')	6.056023	0.001388	-0.038668
H81(C19)	-10.099130	-3.430384	-1.074066
H82(C19)	-10.088598	-3.508713	0.685992
H83(C19)	-8.975238	-4.521970	-0.247322
H84(C19')	8.751408	-3.014577	0.766383
H85(C19')	7.328914	-3.538412	-0.140799
H86(C19')	8.764509	-2.962191	-0.994569
H87(C11)	-6.136306	-0.818116	-0.090148
H88(C11')	5.354796	-3.015230	-0.140826
H89(C12)	-4.511217	-3.416050	-0.201523
H90(C12')	3.721791	-0.420726	-0.059780
H91(C14)	-2.281312	-3.244528	-0.188520
H92(C14')	1.493412	-0.596407	-0.072161
H93(C20)	-2.684745	0.490620	-0.034410
H94(C20)	-4.202630	0.262499	0.838672
H95(C20)	-4.203742	0.337215	-0.921990
H96(C20')	3.416142	-4.170467	0.686855
H97(C20')	1.902874	-4.330787	-0.208793
H98(C20')	3.425208	-4.106011	-1.075062
H99(C15)	-0.893953	-0.475903	-0.072308
H100(C15')	0.108914	-3.366715	-0.183134

Table 7. 9NEO Cartesian coordinates.

Atom	X	Y	Z
O01	-11.186779	-4.860248	0.060083
O01'	12.530945	-2.598575	-0.499931
O02	-7.871158	-2.367914	1.194122
O02'	8.456565	-1.815309	-0.179568
C18'	9.075509	-1.239131	-2.514718
C06'	9.563872	-0.932464	0.039454
C01	-9.563043	-1.752813	-1.320732
C01'	10.445152	-1.324149	1.239993
C02	-10.518815	-2.949810	-1.149904
C02'	10.834229	-2.813956	1.164186
C03	-10.196565	-3.840366	0.035549
C03'	11.331703	-3.296919	-0.186486
C04	-10.208686	-3.021716	1.320367
C04'	10.266437	-3.101052	-1.262812
C05	-9.209341	-1.856184	1.294798
C05'	9.492893	-1.797100	-1.177927
C06	-9.433335	-1.023195	0.026632
C07	9.236776	0.515953	-0.063143
C07	-9.509905	0.279641	0.114353
C08	-9.576095	1.592858	0.206177
C08'	7.978115	0.992515	-0.083179
C09	-8.448932	2.530571	0.132697
C09'	7.610310	2.393232	-0.163354
C10	-7.163520	2.084508	0.128908
C10'	6.309410	2.807929	-0.169534
C11	-5.970195	2.870337	0.048365
C11'	5.124813	2.004586	-0.100908
C12	-4.722522	2.325246	0.059589
C12'	3.873495	2.539068	-0.115349
C13	-3.478925	3.043940	-0.016060
C13'	2.634061	1.811737	-0.047666
C14	-2.309994	2.328151	0.008814
C14'	1.462292	2.522245	-0.073865
C15	-0.976041	2.823874	-0.049800
C15'	0.129571	2.022498	-0.017292

Supplementary material

C16	-8.178543	-2.223268	-1.803267
C16’	9.618046	-1.123275	2.517753
C17	-10.147646	-0.822546	-2.386613
C17’	11.694169	-0.432154	1.312662
C18	-9.327640	-1.027674	2.569398
C19	-8.843578	3.978619	0.070621
C19’	8.711364	3.413179	-0.238400
C20	-3.523991	4.542627	-0.117348
C20’	2.688442	0.313385	0.049043
H45(C04’)	10.736953	-3.185102	-2.251835
H46(C04’)	9.531899	-3.915058	-1.202964
H47(C02’)	11.600415	-3.014950	1.922209
H48(C02’)	9.958554	-3.421889	1.421118
H49(C03’)	11.549620	-4.374685	-0.106624
H50(C18’)	8.489678	-1.986833	-3.062641
H51(C18’)	9.956797	-0.995974	-3.119146
H52(C18’)	8.470639	-0.338456	-2.401671
H53(C07’)	10.085239	1.194143	-0.104187
H54(C17’)	12.259382	-0.449391	0.378861
H55(C17’)	12.358519	-0.793904	2.105183
H56(C17’)	11.428101	0.601315	1.558572
H57(C16’)	10.192271	-1.442760	3.395458
H58(C16’)	8.693916	-1.709442	2.480124
H59(C16’)	9.347922	-0.070960	2.654123
H60(O01’)	12.856476	-2.944332	-1.342955
H61(C08’)	7.179752	0.256079	-0.038788
H62(C19’)	8.309769	4.428391	-0.296740
H63(C19’)	9.348504	3.250753	-1.117330
H64(C19’)	9.366483	3.359489	0.640785
H65(C10’)	6.135238	3.882831	-0.232130
H66(C11’)	5.233349	0.925312	-0.032769
H67(C02)	-10.515757	-3.552860	-2.066212
H68(C02)	-11.545500	-2.582048	-1.015441
H69(C03)	-9.199002	-4.284934	-0.096371
H70(C04)	-9.978315	-3.663112	2.186316
H71(C04)	-11.224513	-2.635240	1.473604
H72(C16)	-8.282098	-2.765737	-2.751224
H73(C16)	-7.527536	-1.359671	-1.975400
H74(C16)	-7.683887	-2.868339	-1.075839
H75(C17)	-10.257793	-1.364447	-3.332891
H76(C17)	-11.133108	-0.446030	-2.092116
H77(C17)	-9.495594	0.038736	-2.563081
H78(C18)	-10.324648	-0.591062	2.676779
H79(C18)	-8.591043	-0.220225	2.571925
H80(C18)	-9.145430	-1.667711	3.442425
H81(C12’)	3.786191	3.624473	-0.183710
H83(O01)	-10.965462	-5.464514	0.782768
H84(C08)	-10.561105	2.042581	0.347865
H85(C20’)	1.697958	-0.141541	0.094556
H86(C20’)	3.211771	-0.114486	-0.814607
H87(C20’)	3.240240	0.000054	0.943569
H88(C14’)	1.551565	3.607262	-0.146262
H89(C19)	-9.498878	4.236600	0.912643
H90(C19)	-7.988659	4.656235	0.096952
H91(C19)	-9.411217	4.190480	-0.844971
H92(C10)	-7.017940	1.005460	0.196056
H93(C15’)	-0.025562	0.947333	0.056382
H94(C11)	-6.067992	3.950730	-0.027313
H95(C15)	-0.818746	3.898811	-0.123777
H96(C12)	-4.644193	1.239821	0.132446
H97(C14)	-2.403776	1.243807	0.083455
H98(C20)	-2.531134	4.991698	-0.167872
H99(C20)	-4.076443	4.856107	-1.011508
H100(C20)	-4.041556	4.976288	0.746990

Table 8. NEO Cartesian coordinates.

Atom	X	Y	Z
O01	13.807685	-2.293649	0.447959
O01’	-13.230447	-2.426125	-0.761408
O02	9.807461	-2.171010	-1.126473
O02’	-10.906033	0.968589	-0.114728
C01	10.571114	-0.651109	1.460017
C01’	-11.344618	-1.118065	1.175698
C02	12.049033	-1.087688	1.454057
C02’	-12.856180	-0.867176	1.006429
C03	12.417761	-2.024327	0.318849
C03’	-13.403999	-1.061943	-0.396094
C04	12.099716	-1.369739	-1.019465
C04’	-12.721273	-0.120504	-1.385935
C05	10.619374	-0.986622	-1.160224
C05’	-11.227195	0.061198	-1.184002
C06	10.191318	-0.154468	0.054979
C06’	-10.550301	-0.407946	0.063899
C07	9.513612	0.949818	-0.124096
C07’	-9.087068	-0.679470	0.055485
C08	8.818843	2.055237	-0.305352
C08’	-8.152370	0.285629	0.141777
C09	7.356713	2.161418	-0.381756

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C09’	-6.716055	0.086098	0.162010	H66(C11’)	-3.936938	0.298841	0.264529
C10	6.575136	1.048934	-0.442275	H67(C02)	12.291762	-1.566373	2.410710
C10’	-5.914970	1.187346	0.256434	H68(C02)	12.692559	-0.200920	1.370745
C11	5.147006	0.992542	-0.499456	H69(C03)	11.841890	-2.957465	0.407316
C11’	-4.486403	1.236765	0.299668	H70(C04)	12.368689	-2.042619	-1.849664
C12	4.456678	-0.177746	-0.572603	H71(C04)	12.725432	-0.473858	-1.122513
C12’	-3.792980	2.403352	0.402072	H72(C16)	9.951617	-2.190056	2.860738
C13	3.021349	-0.359211	-0.612176	H73(C16)	8.617553	-1.480908	1.930253
C13’	-2.358373	2.587292	0.439268	H74(C16)	9.693754	-2.644501	1.157078
C14	2.152665	0.634346	-0.249288	H75(C17)	10.705926	0.104450	3.483103
C14’	-1.488674	1.597027	0.069698	H76(C17)	11.028421	1.334333	2.245164
C15	0.729344	0.599529	-0.294155	H77(C17)	9.367149	0.802027	2.553960
C15’	-0.065467	1.633926	0.112765	H78(C18)	10.959439	0.665590	-2.541705
C16	9.657051	-1.820273	1.870738	H79(C18)	9.323101	-0.021927	-2.602111
C16’	-11.034737	-2.622866	1.190090	H80(C18)	10.691551	-0.905175	-3.314348
C17	10.407330	0.466833	2.492802	H81(C12’)	-4.382290	3.317562	0.492640
C17’	-10.920231	-0.511335	2.520590	H83(O01)	14.047117	-2.929571	-0.240997
C18	10.382500	-0.261570	-2.480543	H84(C08)	9.370799	2.992183	-0.404866
C18’	-10.455507	0.285663	-2.459409	H85(C20’)	-0.850309	4.142565	0.674143
C19	6.831223	3.568489	-0.387793	H86(C20’)	-2.498294	4.732593	0.449187
C19’	-6.193579	-1.318727	0.080245	H87(C20’)	-2.020156	4.044438	1.997334
C20	2.559870	-1.716211	-1.074139	H88(C14’)	-1.916984	0.670367	-0.311722
C20’	-1.896664	3.940992	0.911349	H89(C19)	7.298315	4.150771	-1.192541
H45(C04’)	-12.913327	-0.475044	-2.407729	H90(C19)	5.750199	3.620803	-0.526550
H46(C04’)	-13.177442	0.875960	-1.316816	H91(C19)	7.074420	4.081039	0.552184
H47(C02’)	-13.399702	-1.521471	1.698210	H92(C10)	7.089266	0.086815	-0.447311
H48(C02’)	-13.077459	0.166432	1.298047	H93(C15’)	0.423406	2.527893	0.496740
H49(C03’)	-14.480700	-0.825485	-0.379514	H94(C11)	4.593379	1.929043	-0.495591
H50(C18’)	-10.867603	1.148755	-2.995841	H95(C15)	0.239812	-0.294573	-0.677193
H51(C18’)	-10.539886	-0.587909	-3.115855	H96(C12)	5.046664	-1.093733	-0.633331
H52(C18’)	-9.399285	0.472045	-2.260620	H97(C14)	2.582283	1.560834	0.130983
H53(C07’)	-8.795968	-1.725069	-0.005369	H98(C20)	1.507809	-1.908692	-0.855667
H54(C17’)	-11.211441	-3.082174	0.215636	H99(C20)	2.705823	-1.835530	-2.155669
H55(C17’)	-11.686861	-3.125598	1.912811	H100(C20)	3.147912	-2.504182	-0.588706
H56(C17’)	-10.001230	-2.811043	1.499644				
H57(C16’)	-11.504676	-0.951845	3.337045				
H58(C16’)	-11.081939	0.571639	2.527953				
H59(C16’)	-9.860476	-0.697918	2.723088				
H60(O01’)	-13.619164	-2.542944	-1.639728				
H61(C08’)	-8.502622	1.315428	0.201139				
H62(C19’)	-5.103857	-1.367258	0.103464				
H63(C19’)	-6.529883	-1.806382	-0.843267				
H64(C19’)	-6.571982	-1.923284	0.913950				
H65(C10’)	-6.417229	2.154410	0.307717				

Supplementary material

1. Chemical reactivity indexes.

2.1 Electronegativity (χ). It is equivalent to the chemical potential (μ) negative value. It is calculated starting with the ionization potential (*I*) and electronic affinity (*A*) with the next working equation [36]:

$$\chi = \frac{I+A}{2} = -\mu \quad (5)$$

As we will see when talking about the electrophilicity index, electronegativity is conceived as a kind of driving force that favors electronic transfer.

2.2 Hardness (η). It is converse to the softness (*S*), this value may be calculated using the following working equation [37]:

$$\eta = \frac{I-A}{2} = \frac{1}{S} \quad (6)$$

2.3 Electrophilicity index (ω). It is defined as energy released by an acceptor molecule once it gets saturated with electrons, the working equation to calculate this index is:

$$\omega = \frac{\chi^2}{2\eta} \quad (7)$$

This last equation is analogous to the equation used in basic electricity to relate electric power (*W*) with voltage (*V*) and resistance (*R*):

$$W = \frac{V^2}{R} \quad (8)$$

An important characteristic of this property is that it is well described in gas phase, when the donor and acceptor molecules are close enough for electronic transfer, since solvent molecules have been removed and are irrelevant [38].

2.4 Electrodonor power (ω-) and electroacceptor power (ω+). The next working equations are used to calculate these values [39]:

$$\omega^- = \frac{(3I+A)^2}{16(I-A)} \quad (9)$$

$$\omega^+ = \frac{(I+3A)^2}{16(I-A)} \quad (10)$$

In order to compare ω+ with ω- the following working equation for net electrophilicity has been proposed [40]:

$$\Delta\omega^{\pm} = \omega^+ - (-\omega^-) = \omega^+ + \omega^- \quad (11)$$

2.5 Condensed Fukui functions. They play a crucial role in the relationship between frontier molecular orbital theory and the principles for acids and basis (soft and hard) [41]. Condensed Fukui functions are based in the concept of integrate them in atomic regions, this procedure is like that used on the techniques to analyze populations [42]; when such integration is combined with the finite difference approximation the next equations can be obtained:

$$f_k^+ = q_k(N+1) - q_k(N) \quad (12)$$

$$f_k^- = q_k(N) - q_k(N-1) \quad (13)$$

$$f_k^0 = \frac{q_k(N+1) + q_k(N-1)}{2} \quad (14)$$

Where f_k^+, f_k^- and f_k^0 are condensed Fukui function values for atoms subject to a nucleophilic attack, an electrophilic attack and a radical attack, respectively. $q_k(N)$ denotes the electronic population of atom *k* of the neutral molecule, $q_k(N+1)$ denotes the electronic population of atom *k* of the anion and $q_k(N-1)$ denotes the electronic population of atom *k* of the cation. In the literature, negative values have been reported when using equations (12), (13) y (14), It is unknown if these negative values have physical interpretation. The presence of these negative values has been attributed to relaxation effects and to inadequate charge partition techniques [43]. Atomic population value is sensitive to partition scheme, in this work, Hirshfeld partition technique was used because it is considered superior to other options despite of getting a few negative values [44].

2.6 Condensed dual descriptor. It is another local reactivity descriptor ($f^{(2)}(r)$). This descriptor possesses the capability to locate atoms prone to nucleophilic and electrophilic attacks more efficiently than condensed Fukui functions and

with less ambiguity. The following working equation is as shown next [45]:

$$f^{(2)}(r) = f^{+}_{(k)} - f^{-}_{(k)} \quad (15)$$

2.7 Condensed local softness. Condensed Fukui function values can be compared only within the same molecule. However, when the condensed Fukui function value is multiplied by the global molecular softness (*S*) one can obtain the condensed local softness (e.g. $s^{+}_{(k)}$) and the values obtained in this manner permit us to compare atom susceptibility in different molecules to nucleophilic, electrophilic, and radical attacks [46]. The next working equations to calculate these values are:

$$s^{+}_{(k)} = f^{+}_{(k)}\ multiplied\ by\ S \quad (16)$$

$$s^{-}_{(k)} = f^{-}_{(k)}\ multiplied\ by\ S \quad (17)$$

$$s^{0}_{(k)} = f^{0}_{(k)}\ multiplied\ by\ S \quad (18)$$

2.8 Intramolecular reorganization energy. It is defined as the sum of two identical energies, the first one is the required energy to pass from neutral molecule Geometry to ionized molecule Geometry (as a cation due to the loss of charge or as anion due to the acceptance of charge). The second energy is the inverse process, the relaxation of an ion Geometry to neutral molecule; all of this governed by charge transfer process principles.

Intramolecular reorganization energy is obtained through 2 terms that come from structural relaxing energies in their neutral and charged forms. Total adiabatic reorganization energy can be calculated with a working equation (19), which in turn may be calculated with the following working equations (16) and (17):

$$\lambda_{tot} = \lambda_N + \lambda_C \quad (19)$$

$$\lambda_N = E_N\,(rel) - E_N \quad (20)$$

$$\lambda_C = E_C - E_C\,(rel) \quad (21)$$

Where λ_N is the neutral molecular reorganization energy, E_N *(rel)* is the molecular neutral energy acquired from an anion or cation optimized molecular Geometry, E_N is the neutral molecular energy obtained from a neutral molecular Geometry, λ_C is the reorganization energy of the molecule in charged state (anion or cation) acquired from an optimized Geometry of the charged molecule, E_C is the charged molecular energy obtained from an optimized Geometry of a neutral molecule and E_C*(rel)* is the charged molecule energy (cation or anion) acquired from an optimized Geometry of a molecule in its anionic or cationic state.

2.9 Electron and hole extraction potentials. Reorganization energies are related with the hole and electron extraction potentials with the next working equations (22) and (23).

$$HEP = IP - \lambda_h \quad (22)$$

$$EEP = EA + \lambda_e \quad (23)$$

Where *HEP* is the hole extraction potential, *EEP* is the electron extraction potential, λ_h is the hole reorganization energy and λ_e is the electron reorganization energy. λ_h and λ_e correspond to cationic λ_{tot} and anionic λ_{tot}, respectively.

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