Predicting Reactive Sites with Quantum Chemical Topology: Carbonyl Additions in Multicomponent Reactions

David Ramirez-Palma,[a] César R. García-Jacas,[b]
Pablo Carpio-Martinez,[c] Fernando Cortés-Guzmán*[a]

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Table 1: Carbonyl structures and their hydration equilibrium constants

ID	Molecule	$logk$
1	H_2CO	3.36
2	$(CH_3)_2CO$	-2.85
3	$ClCH_2COCH_3$	-1.05
4	$3Cl-PhCHO$	-1.66
5	CH_3CH_2CHO	-0.07
6	$(CH_3)_2CHCHO$	-0.21
7	CCl_3CHO	4.45
8	$4Cl-PhCHO$	-1.79
9	$4CF_3-PhCHO$	-1.25
10	$3NO_2-PhCHO$	-0.96
11	$4Cl,3NO_2-PhCHO$	-0.74
12	$3,5(NO_2)_2-PhCHO$	0.32
13	$2Cl,5NO_2-PhCHO$	-0.47
14	FCH_2COCH_3	-0.78
15	CF_3COCH_3	1.54
16	$(CH_3)_2CHCOOCH_3$	-10.42
17	$PhCOCF_3$	1.89
18	$ClCH_2COOCH_3$	-6.66
19	CF_3COOCH_3	-0.9
20	CHF_2COOCH_3	-2.92
21	$CH_3CON(CH_3)_2$	-14.2
22	$HCOOCH_3$	-6.6
23	$HCON(CH_3)_2$	-13.8
24	$CH_3CH_2COOCH_3$	-9.43
25	$CH_3OCH_2COOCH_3$	-9.21
26	$PhCOCHCl_2$	-0.48
27	CCl_3COOCH_3	-4.24
28	$CF_3CON(CH_3)_2$	-9.2
29	CH_3CHO	0.03
30	$ClCH_2COCH_2Cl$	1
31	$CH_3CH_2CH_2CHO$	-0.08
32	$(CH_3)_3CCHO$	-0.63
33	$3,4Cl_2-PhCHO$	-1.35
34	$4NO_2-PhCHO$	-0.77
35	$CHCl_2COCH_3$	0.46
36	CH_3COOCH_3	-8.2
37	$CHCl_2COOCH_3$	-4.34
38	$PhCOOCH_3$	-10.07
39	$HCON(CH_3)Ph$	-10.22
40	$PhCOCH_3$	-5.18

Table 2: Electrostatic descriptors of carbon atom in the carbonyl group

ID	$q(C)$	$\|\mu(C)\|$	$\mu_X(C)$	$\mu_Y(C)$	$\mu_Z(C)$	$Q_{XX}(C)$	$Q_{YY}(C)$	$Q_{ZZ}(C)$	$Q_{EigVal1}(C)$	$Q_{EigVal2}(C)$	$Q_{EigVal3}(C)$	$\|Q(C)\|$
1	1.127860	0.038030	-0.000012	0.000025	0.038030	-1.411130	0.020714	1.390416	-1.411130	0.020714	1.390416	1.617606
2	1.103553	0.119170	0.101434	-0.060377	-0.016351	0.978734	-0.001909	-0.976825	-1.350208	-0.063781	1.413989	1.129044
3	1.077850	0.112827	0.112346	-0.000766	0.010378	1.362633	-0.112076	-1.250558	-1.279146	-0.108342	1.387488	1.512884
4	1.092619	0.139402	0.026366	-0.136577	0.009185	1.048296	0.215045	-1.263341	-1.273794	-0.046510	1.320303	1.351838
5	1.110687	0.042984	0.032614	-0.003706	-0.027753	0.215026	-0.059347	-0.155679	-1.264099	-0.063517	1.327616	0.222102
6	1.103388	0.114368	-0.054253	0.099306	0.016579	-0.952373	0.043030	0.909342	-1.578267	0.037904	1.540363	1.075723
7	1.090414	0.134736	0.033382	-0.127794	-0.026615	0.183433	0.040454	-0.223887	-1.351688	-0.072973	1.424662	0.238620
8	1.090133	0.136228	0.033952	-0.130335	-0.020446	-0.421650	0.109723	0.311928	-1.351500	-0.074799	1.426299	0.437513
9	1.083724	0.144738	0.020423	-0.142610	0.013946	-0.806248	0.166307	0.639940	-1.306223	-0.143587	1.449809	0.851359
10	1.079670	0.152651	0.069752	-0.135599	-0.007079	0.311692	0.908519	-1.220212	-1.226927	-0.222999	1.449926	1.267932
11	1.193420	0.089412	-0.030892	0.082987	0.012383	-0.808401	0.298460	0.509941	-1.314856	-0.132217	1.447074	0.817570
12	1.099143	0.129040	-0.052179	0.118019	-0.000134	1.477129	0.076739	-1.553868	-1.591042	0.046107	1.544934	1.751629
13	1.105224	0.107545	-0.040617	0.099580	-0.000120	1.467236	0.080302	-1.547537	-1.578167	0.045576	1.532591	1.742431
14	1.046028	0.103861	-0.058762	-0.084943	0.010899	1.513142	-0.091586	-1.421556	-1.609669	0.000529	1.609140	1.696822
15	1.110891	0.089677	-0.056955	0.069195	-0.003181	0.264241	1.235864	-1.500105	-1.571393	0.042924	1.528469	1.601561
16	1.107233	0.086654	-0.024198	0.083143	-0.003251	1.341391	0.079469	-1.420860	-1.564058	0.039070	1.524988	1.596765
17	1.111308	0.083749	-0.049736	0.067351	0.002012	0.267894	1.290773	-1.558668	-1.565760	0.043227	1.522533	1.666795
18	1.121698	0.045512	-0.007971	0.044656	0.003690	1.441293	0.070230	-1.511523	-1.549373	0.045161	1.504212	1.706255
19	1.112823	0.065261	-0.019216	0.062191	0.004694	1.390149	0.080920	-1.471069	-1.542634	0.053701	1.488933	1.653906
20	1.117930	0.177852	-0.029392	-0.171691	0.035914	0.987671	0.051969	-1.039640	-1.249421	-0.071778	1.321199	1.171622
21	1.082706	0.159008	0.045606	-0.152031	-0.009494	1.022397	0.207039	-1.229435	-1.281448	-0.084827	1.366274	1.316478
22	1.141228	0.249212	-0.092779	-0.227380	0.042389	0.995756	-0.062152	-0.933604	-1.261258	-0.091869	1.353128	1.115649
23	1.570193	0.281089	-0.032960	0.250029	0.124137	0.008251	0.894102	-0.902354	-1.511041	-0.152104	1.663145	1.037217
24	1.591960	0.271614	0.004756	-0.271569	0.001384	0.113508	1.469108	-1.582616	-1.582658	-0.073265	1.655923	1.765566
25	1.686233	0.284262	0.040855	0.000520	-0.281310	-0.004888	-1.592979	1.597867	-1.592981	-0.026664	1.619644	1.842242
26	1.075460	0.130231	-0.130062	-0.006624	-0.000045	0.163532	1.412284	-1.575815	-1.575816	0.133971	1.441845	1.732913
27	1.586231	0.277519	0.069820	-0.268592	0.000267	0.046018	1.699463	-1.745480	-1.745487	0.035596	1.709891	1.989471
28	1.639371	0.238992	-0.101278	-0.216471	0.000035	0.265015	1.339127	-1.604143	-1.604143	-0.051741	1.655884	1.719839
29	1.713959	0.302015	-0.204977	-0.221805	0.000176	0.003944	1.594795	-1.598740	-1.598740	-0.044771	1.643511	1.843793
30	1.666618	0.294034	-0.095923	-0.277537	-0.015093	-0.103111	1.648873	-1.545762	-1.551457	-0.103392	1.654849	1.847303
31	1.455904	0.320302	-0.209386	0.240342	-0.031406	0.846285	0.905079	-1.751364	-1.762994	0.094603	1.668391	1.751693
32	1.634796	0.252822	0.220533	0.123628	-0.000294	0.968703	0.676665	-1.645368	-1.645369	-0.137408	1.782777	1.653984
33	1.498701	0.353698	0.335794	0.111106	0.000272	1.867029	0.001973	-1.869002	-1.869003	0.001054	1.867949	2.156999
34	1.486494	0.223967	-0.151521	0.159094	-0.043494	0.104775	1.563708	-1.668483	-1.863270	-0.027424	1.890694	1.869045
35	1.580275	0.276515	-0.016227	-0.276038	-0.000079	0.226964	1.343937	-1.570901	-1.570901	-0.108497	1.679398	1.698118
36	1.617347	0.229038	-0.042239	-0.225110	0.000007	0.083196	1.503868	-1.587064	-1.587064	-0.086437	1.673502	1.786489
37	1.023810	0.124229	0.047399	0.114831	0.000237	0.331627	1.200281	-1.531908	-1.531922	0.059959	1.471963	1.611913
38	1.053642	0.114838	-0.091852	-0.068927	-0.000033	0.157608	1.397124	-1.554731	-1.554732	0.155542	1.399190	1.711526
39	1.722389	0.284570	-0.181696	-0.219012	-0.000414	0.067178	1.546229	-1.613407	-1.613407	-0.005370	1.618777	1.825453
40	1.554695	0.318272	-0.228410	0.221275	0.012783	0.488539	1.307806	-1.796345	-1.797631	0.176404	1.621227	1.857576

Table 3: Delocalization and energetic descriptors of carbon atom in the carbonyl group

ID	$\lambda(C)$	$\delta_{Bond}(C,A)/2$	$\delta_{NonBond}(C,A)/2$	$K_{Scaled}(C)$	$V_{en}(C)$
1	3.230046	1.642101	-0.000007	-37.289000	-105.029835
2	3.188859	1.640051	0.067536	-37.322300	-117.162290
3	3.162857	1.634810	0.124483	-37.347230	-129.212816
4	3.152900	1.621549	0.132933	-37.187864	-143.967944
5	3.133848	1.610888	0.144577	-37.164354	-159.234230
6	3.178329	1.634494	0.083788	-37.208756	-149.726303
7	3.200014	1.627767	0.081805	-37.344577	-124.870660
8	3.199794	1.628360	0.081714	-37.347345	-129.945004
9	3.204043	1.612586	0.099647	-37.363377	-132.932927
10	3.204768	1.597013	0.118549	-37.378417	-141.092521
11	3.115293	1.574726	0.116561	-37.092245	-161.227892
12	3.179983	1.636357	0.084517	-37.211422	-148.806235
13	3.176336	1.635155	0.083285	-37.172620	-156.739924
14	3.211685	1.659365	0.082922	-37.377379	-156.460632
15	3.173059	1.634969	0.081080	-37.318808	-152.268634
16	3.177581	1.634550	0.080636	-37.321368	-150.980666
17	3.173105	1.634767	0.080820	-37.222889	-159.372528
18	3.167277	1.633431	0.077594	-37.305161	-162.745361
19	3.175447	1.627148	0.084582	-37.221002	-165.444148
20	3.128453	1.602526	0.151091	-37.154603	-159.117920
21	3.165272	1.613363	0.138659	-37.347921	-138.023178
22	3.120203	1.574800	0.163769	-37.308045	-154.361767
23	2.825012	1.498601	0.106193	-37.094364	-146.986187
24	2.804862	1.523017	0.080161	-37.053850	-132.467298
25	2.716046	1.498303	0.099419	-36.978970	-158.433229
26	3.143615	1.602715	0.178210	-37.392633	-180.504466
27	2.801063	1.522150	0.090557	-37.063640	-154.957295
28	2.761306	1.513557	0.085767	-37.005540	-145.420114
29	2.703898	1.468291	0.113853	-36.990014	-154.260331
30	2.746192	1.483769	0.103421	-37.025451	-147.403250
31	2.856765	1.587825	0.099506	-37.165375	-140.352324
32	2.820879	1.524102	0.020223	-37.010607	-121.067204
33	2.867447	1.583125	0.050727	-37.135291	-128.882999
34	2.877143	1.578306	0.058056	-37.147454	-146.867946
35	2.816852	1.510213	0.092660	-37.075041	-139.639329
36	2.786059	1.500161	0.096433	-37.053868	-144.692422
37	3.181761	1.658889	0.135540	-37.419875	-155.003056
38	3.151965	1.629587	0.164805	-37.366024	-185.020784
39	2.685034	1.484105	0.108471	-36.949565	-171.012225
40	2.769944	1.541246	0.134115	-37.105835	-162.761899

Table 4: Electrostatic descriptors of oxygen atom in the carbonyl group

ID	$q(O)$	$\|\mu(O)\|$	$\mu_X(O)$	$\mu_Y(O)$	$\mu_Z(O)$	$Q_{XX}(O)$	$Q_{YY}(0)$	$Q_{ZZ}(0)$	$Q_{EigVal1}(O)$	$Q_{EigVal2}(O)$	$Q_{EigVal3}(O)$	$\|Q(O)\|$
1	-1.149522	1.180646	-0.000002	0.000000	-1.180646	-0.076664	-0.291394	0.368058	-0.291394	-0.076664	0.368058	0.388377
2	-1.179307	1.249199	1.023941	0.596323	0.395526	0.247115	-0.133492	-0.113623	-0.281574	-0.151036	0.432610	0.247381
3	-1.199748	1.310584	1.304136	0.006016	0.129712	0.445633	-0.217937	-0.227696	-0.234616	-0.217767	0.452383	0.445669
4	-1.189916	1.278772	1.120775	-0.612289	0.064989	0.317057	-0.103293	-0.213764	-0.217435	-0.211531	0.428966	0.323409
5	-1.164849	1.219013	0.921041	-0.109845	-0.790955	0.144305	-0.204753	0.060448	-0.210406	-0.170851	0.381257	0.210399
6	-1.169519	1.243867	-0.448313	0.576524	-1.006896	-0.090334	-0.025547	0.115881	-0.204545	-0.174126	0.378671	0.121768
7	-1.183586	1.258593	0.934269	-0.481097	0.692636	0.098514	-0.040509	-0.058005	-0.215105	-0.160486	0.375591	0.099031
8	-1.183382	1.258814	0.729527	-0.529013	0.878948	-0.018049	-0.024260	0.042310	-0.212881	-0.162688	0.375569	0.042461
9	-1.184010	1.255187	0.566891	-0.590789	-0.951366	-0.107429	0.014647	0.092782	-0.226774	-0.146970	0.373744	0.116516
10	-1.185881	1.253356	-0.705663	-1.034134	-0.059241	-0.028905	0.258656	-0.229751	-0.231292	-0.137989	0.369281	0.283460
11	-1.142982	1.103287	0.466618	-0.509324	-0.860290	-0.047361	0.001419	0.045942	-0.149688	-0.118299	0.267987	0.053887
12	-1.172348	1.255019	-1.243834	0.106204	0.129117	0.362088	-0.183486	-0.178602	-0.205941	-0.183835	0.389776	0.362099
13	-1.167698	1.241052	-1.231113	0.104483	0.116851	0.352203	-0.183139	-0.169064	-0.206373	-0.173244	0.379617	0.352297
14	-1.113290	1.222328	-1.199389	0.050595	-0.230201	0.481157	-0.290444	-0.190713	-0.296996	-0.205453	0.502449	0.484590
15	-1.161747	1.221079	0.567814	1.065094	-0.184923	-0.135649	0.282019	-0.146370	-0.210710	-0.157810	0.368519	0.282087
16	-1.161132	1.223001	-1.188354	0.152471	0.245559	0.310975	-0.167044	-0.143931	-0.200943	-0.160911	0.361854	0.311261
17	-1.162738	1.226610	0.573402	1.082817	0.057337	-0.136292	0.299393	-0.163102	-0.206549	-0.164310	0.370859	0.299793
18	-1.152214	1.194124	-1.186517	0.062309	0.119272	0.323228	-0.186672	-0.136556	-0.206822	-0.142058	0.348880	0.324520
19	-1.155377	1.214815	-1.199109	0.059783	0.185307	0.310513	-0.151686	-0.158827	-0.172052	-0.169641	0.341692	0.310540
20	-1.172559	1.227745	1.038668	-0.546986	0.359629	0.246101	-0.126704	-0.119396	-0.218939	-0.163179	0.382119	0.246137
21	-1.197354	1.292709	1.125763	-0.610422	-0.176464	0.329067	-0.138984	-0.190083	-0.261798	-0.202313	0.464111	0.330387
22	-1.144202	1.153769	0.989819	-0.436459	0.401179	0.189785	-0.071094	-0.118690	-0.175380	-0.122158	0.297538	0.191764
23	-1.195460	1.352707	-0.231471	1.161557	0.653469	0.028149	0.275067	-0.303216	-0.548410	0.030892	0.517518	0.335056
24	-1.193394	1.345682	0.169580	-1.334950	-0.003516	-0.107390	0.579549	-0.472160	-0.472167	-0.111612	0.583780	0.616628
25	-1.164204	1.283206	-0.661349	-0.000359	-1.099652	0.032593	-0.412137	0.379544	-0.412137	-0.164305	0.576442	0.458238
26	-1.090683	1.171016	-0.284762	-1.135865	0.000018	-0.036527	0.349677	-0.313150	-0.313150	-0.068666	0.381817	0.384423
27	-1.188778	1.354768	0.535223	-1.244562	-0.000063	0.071888	0.458042	-0.529931	-0.529931	0.013596	0.516335	0.574919
28	-1.175132	1.279603	-0.000320	-1.279603	-0.000049	-0.030226	0.511663	-0.481437	-0.481437	-0.033306	0.514743	0.574163
29	-1.143142	1.216211	0.309406	-1.176196	-0.000053	-0.072729	0.485030	-0.412300	-0.412300	-0.095818	0.508118	0.523154
30	-1.164961	1.282914	0.518553	-1.172541	-0.046019	-0.072334	0.477372	-0.405038	-0.406499	-0.189929	0.596428	0.514569
31	-1.201112	1.455546	-0.422031	1.392011	-0.053004	-0.012261	0.631697	-0.619436	-0.623074	-0.072734	0.695808	0.722446
32	-1.178487	1.298412	0.528352	1.186052	0.000005	-0.015356	0.389943	-0.374587	-0.374587	-0.219405	0.593992	0.441669
33	-1.193216	1.409045	1.269750	-0.610854	0.000198	0.607021	-0.116672	-0.490348	-0.490348	-0.250508	0.740857	0.644219
34	-1.177362	1.270816	0.036841	1.224841	-0.336719	-0.107137	0.527525	-0.420388	-0.526580	-0.080735	0.607316	0.557666
35	-1.195069	1.351889	0.039128	-1.351323	-0.000028	0.017685	0.516121	-0.533806	-0.533806	0.017352	0.516454	0.606434
36	-1.171592	1.279102	0.192023	-1.264606	-0.000009	-0.018847	0.499889	-0.481042	-0.481042	-0.020913	0.501955	0.566654
37	-1.140875	1.305699	0.566952	1.176186	0.000058	-0.036907	0.391544	-0.354637	-0.354637	-0.148628	0.503264	0.432386
38	-1.114576	1.239566	-0.074368	-1.237333	-0.000015	-0.131898	0.449315	-0.317417	-0.317417	-0.132564	0.449982	0.461905
39	-1.154327	1.234642	0.265341	-1.205793	0.000066	0.002243	0.462738	-0.464981	-0.464981	-0.008455	0.473436	0.535624
40	-1.156324	1.332521	0.003697	1.332468	0.011273	0.003397	0.596134	-0.599531	-0.599860	0.002773	0.597087	0.690326

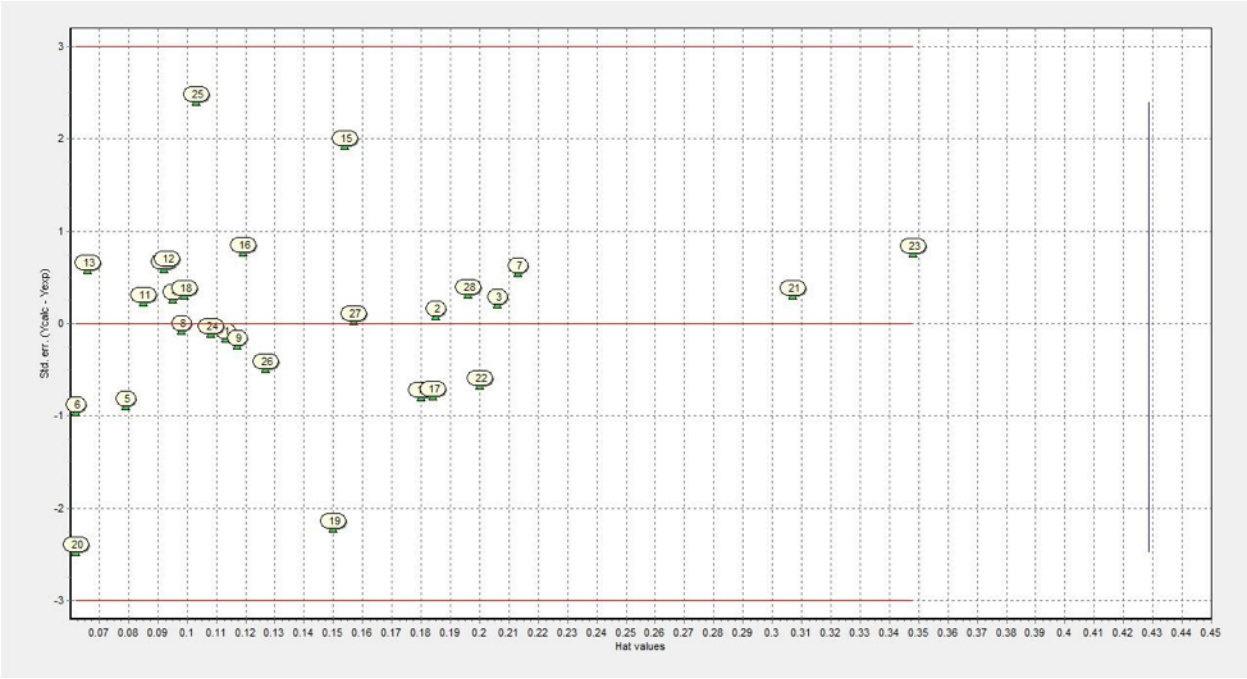

Figure 1: Williams graph for the regression model of 3 variables.

Table 5: Delocalization and energetic descriptors of oxygen atom in the carbonyl group

ID	$\lambda(O)$	$\delta_{Bond}(O,A)/2$	$\delta_{NonBond}(O,A)/2$	$K_{Scaled}(O)$	$V_{en}(O)$	$V_{enO}(O)$
1	8.271619	0.750446	0.127458	-75.922629	-213.566135	-184.148104
2	8.296188	0.715883	0.167236	-75.949537	-228.623517	-184.291458
3	8.308219	0.689973	0.201556	-75.968299	-243.831099	-184.394641
4	8.288003	0.690615	0.211298	-75.648473	-264.069930	-184.371380
5	8.255497	0.698360	0.210992	-75.589616	-285.327766	-184.268373
6	8.264523	0.705081	0.199915	-75.690741	-280.762270	-184.265874
7	8.284062	0.711228	0.188296	-75.961356	-241.895830	-184.317627
8	8.283862	0.711478	0.188043	-75.967855	-250.355997	-184.316833
9	8.282967	0.710431	0.190611	-75.967721	-252.628744	-184.318366
10	8.283339	0.708816	0.193726	-75.972996	-263.678249	-184.329863
11	8.220091	0.724245	0.198646	-75.565286	-297.789600	-184.208129
12	8.267878	0.702953	0.201518	-75.688527	-277.897225	-184.273067
13	8.261745	0.705191	0.200762	-75.618958	-290.206701	-184.258011
14	8.190176	0.728468	0.194646	-75.901097	-288.371872	-184.588198
15	8.254501	0.708293	0.198952	-75.924233	-285.843811	-184.238822
16	8.253191	0.708777	0.199164	-75.923532	-281.883930	-184.234495
17	8.255455	0.707369	0.199915	-75.729413	-294.572678	-184.242286
18	8.241475	0.712549	0.198190	-75.912552	-302.521352	-184.207568
19	8.241413	0.710764	0.203200	-75.728269	-304.488706	-184.218372
20	8.263455	0.693665	0.215439	-75.595305	-286.955711	-184.310132
21	8.304244	0.690056	0.203054	-75.922790	-255.074031	-184.392721
22	8.231432	0.707974	0.204795	-75.888544	-281.706376	-184.211160
23	8.264775	0.633874	0.296811	-75.999747	-284.872019	-185.027196
24	8.281965	0.638448	0.272981	-75.977689	-260.556305	-185.019046
25	8.238043	0.639335	0.286826	-75.889370	-302.918870	-184.898426
26	8.131220	0.713944	0.245519	-75.912837	-319.716679	-184.549829
27	8.255747	0.630245	0.302786	-75.992005	-298.713244	-185.007579
28	8.239289	0.645353	0.290490	-75.920003	-286.129213	-184.970159
29	8.212708	0.651399	0.279035	-75.913606	-297.699381	-184.835877
30	8.246715	0.644306	0.273940	-75.918172	-283.575955	-184.893270
31	8.283844	0.627984	0.289283	-75.972096	-269.150955	-184.983825
32	8.275892	0.657521	0.245074	-75.955519	-245.438617	-184.949760
33	8.294054	0.644248	0.254915	-75.953393	-253.660610	-184.934312
34	8.252149	0.680973	0.244239	-75.983732	-289.867253	-184.918306
35	8.267224	0.634886	0.292959	-75.990424	-273.802476	-185.030018
36	8.245986	0.645858	0.279748	-75.973240	-283.018819	-184.949403
37	8.203727	0.700553	0.236595	-75.976358	-282.091704	-184.717610
38	8.156468	0.701563	0.256544	-75.881061	-324.848183	-184.633239
39	8.200574	0.644640	0.309113	-75.898650	-329.251056	-184.900018
40	8.215100	0.636778	0.304446	-75.900736	-307.002614	-184.846288

Table 6: Experimental and predicted values, and errors in the prediction, for the training and test compounds

ID	Status	Y Exp.	Y-Calc	Y-Pred	Hat	Err.Calc.	Err.Pred.	Std.Err.Calc.	Std.Err.Pred.
1	Training	3.36	3.17	3.15	0.113	-0.19	-0.21	-0.16	-0.19
2	Training	-2.85	-2.75	-2.73	0.185	0.1	0.12	0.09	0.11
3	Training	-1.05	-0.82	-0.77	0.206	0.23	0.28	0.21	0.27
4	Training	-1.66	-1.35	-1.32	0.095	0.31	0.34	0.27	0.3
5	Training	-0.07	-1.1	-1.18	0.079	-1.03	-1.11	-0.89	-0.97
6	Training	-0.21	-1.32	-1.39	0.062	-1.11	-1.18	-0.95	-1.01
7	Training	4.45	5.04	5.2	0.213	0.59	0.75	0.55	0.7
8	Training	-1.79	-1.87	-1.88	0.098	-0.08	-0.09	-0.07	-0.08
9	Training	-1.25	-1.51	-1.54	0.117	-0.26	-0.29	-0.23	-0.26
10	Training	-0.96	-0.28	-0.21	0.092	0.68	0.75	0.59	0.65
11	Training	-0.74	-0.48	-0.45	0.085	0.26	0.29	0.23	0.25
12	Training	0.32	1.04	1.12	0.093	0.72	0.8	0.63	0.7
13	Training	-0.47	0.2	0.25	0.066	0.67	0.72	0.58	0.62
14	Training	-0.78	-1.64	-1.83	0.18	-0.86	-1.05	-0.79	-0.96
15	Training	1.54	3.67	4.06	0.154	2.13	2.52	1.93	2.28
16	Training	-10.42	-9.55	-9.43	0.119	0.87	0.99	0.77	0.87
17	Training	1.89	1.04	0.85	0.184	-0.85	-1.04	-0.78	-0.96
18	Training	-6.66	-6.31	-6.27	0.099	0.35	0.39	0.31	0.34
19	Training	-0.9	-3.35	-3.78	0.15	-2.45	-2.88	-2.21	-2.6
20	Training	-2.92	-5.79	-5.98	0.062	-2.87	-3.06	-2.47	-2.63
21	Training	-14.2	-13.89	-13.76	0.307	0.31	0.44	0.31	0.44
22	Training	-6.6	-7.32	-7.5	0.2	-0.72	-0.9	-0.67	-0.83
23	Training	-13.8	-13.06	-12.66	0.348	0.74	1.14	0.76	1.17
24	Training	-9.43	-9.56	-9.57	0.108	-0.13	-0.14	-0.11	-0.12
25	Training	-9.21	-6.46	-6.15	0.103	2.75	3.06	2.41	2.69
26	Training	-0.48	-1.03	-1.11	0.127	-0.55	-0.63	-0.49	-0.56
27	Training	-4.24	-4.21	-4.2	0.157	0.03	0.04	0.03	0.03
28	Training	-9.2	-8.85	-8.77	0.196	0.35	0.43	0.32	0.4

Table 7: Experimental and predicted values, and errors in the prediction, for the training and test compounds, cont.

ID	Status	Y Exp.	Y-Calc	Y-Pred	Hat	Err.Calc.	Err.Pred.	Std.Err.Calc.	Std.Err.Pred.
29	Test	0.03	-	-0.12	0.101	-	-0.15	-	-
30	Test	1	-	1.63	0.131	-	0.63	-	-
31	Test	-0.08	-	-1.1	0.078	-	-1.02	-	-
32	Test	-0.63	-	-1.29	0.059	-	-0.66	-	-
33	Test	-1.35	-	-1.17	0.088	-	0.18	-	-
34	Test	-0.77	-	-0.34	0.086	-	0.43	-	-
35	Test	0.46	-	1.44	0.141	-	0.98	-	-
36	Test	-8.2	-	-8.59	0.083	-	-0.39	-	-
37	Test	-4.34	-	-5.51	0.053	-	-1.17	-	-
38	Test	-10.07	-	-9.92	0.109	-	0.15	-	-
39	Test	-10.22	-	-8.65	0.352	-	1.57	-	-
40	Test	-5.18	-	-4.4	0.092	-	0.78	-	-

Table 8: Regression coefficients corresponding to the descriptors included in the best model built.

	Variable	Regression Coeff.	Errors Reg.Coeff.	Conf.Intervals (.95)	Std. Reg.Coeff.
-	Intercept	59.4	5.95	12.27	-
1	$Q_{\sigma}(C)$	-9.68	2.4	4.94	-0.27
2	$\|\mu(O)\|$	-35.68	4.54	9.38	-0.55
3	$Q_{\pi}(O)$	8.36	2.47	5.09	0.28

Table 9: Statistical parameters corresponding to the best model built.

R^2	94.68
Q^2	93.11
Q^2_{boot}	92.8
Q^2_{ext}	96.04
$SDEPext$	0.8
$a(R^2)$	0.089
$a(Q^2)$	-0.246
R^2_{adj}	94.02
LOF	2.006
AIC	1.926
K_x	67.13
K_{xy}	76.4
$SDEP$	1.267
$SDEC$	1.113
F	142.44
s	1.202
DF	24
DK	0.093
DQ	0.003
RP	0.005
RN	0
TSS	652.09
AVH	0.143

Table 10: Values of the descriptors of reaction 1

Hep-dio-A	$q(C)$	$\|\mu(CO)\|$	$Q_{EigVal1}(C)$	κ
1	1.0624	1.38523268	-1.210905	-1.05461836
7	1.0596	1.42428618	-1.221972	-2.03982091
11	1.0518	1.37368428	-1.214872	-0.81261386

Table 11: Values of the descriptors of reaction 2

As-A-Me	$q(C)$	$\|\mu(CO)\|$	$Q_{EigVal1}(C)$	κ
7	1.6274	1.36142293	-1.467414	-2.24767095
8	1.6376	1.34740283	-1.497544	-2.12634757

Table 12: Values of the descriptors of reaction 3

X	$q(C)$	$\|\mu(CO)\|$	$Q_{EigVal1}(C)$	κ
1	1.8950	1.7619110	-1.876631	-14.365721
2	1.0525	1.3758467	-1.280461	-1.309882
3	1.6137	1.4935220	-1.582851	-6.111606
4	1.0579	1.2168798	-1.408524	1.520880
5	0.7074	1.2081774	-1.111323	3.748597
6	1.8984	1.3616048	-1.907395	-5.249726
7	1.8337	1.7288674	-1.893144	-13.708443
8	1.0262	1.3037136	-1.178814	1.063117
9	1.6188	1.5809112	-1.449182	-7.236685

Table 13: Values of the descriptors during the reaction between cyclohexanone and Lithium aluminium hydride

	Step	Point	$N(O)$	$q(O)$	$\mu(O)$ $\mu_x(O)$	$\mu_y(O)$	$\mu_Z(O)$	$Q(O)$	$\|\mu(O)\|$	k
	Reactant		9.1641	-1.1641	1.1370	-0.4251	0.0091	-0.2419	1.2139	26.2469
	reactant-Al	-11	9.2560	-1.2560	1.6626	0.1188	0.0144	-0.4053	1.6669	11.4169
	10	-10	9.3130	-1.3130	-0.1027	-0.9167	-0.0045	-0.5878	0.9289	36.2529
	9	-9	9.3143	-1.3143	-0.1237	-0.9134	-0.0045	-0.5992	0.9218	36.6828
	8	-8	9.3158	-1.3158	-0.1446	-0.9107	-0.0046	-0.6108	0.9221	37.0526
	7	-7	9.3174	-1.3174	-0.1680	-0.9085	-0.0046	-0.6244	0.9239	37.4280
	6	-6	9.3190	-1.3190	-0.1926	-0.9068	-0.0046	-0.6392	0.9271	37.7993
R	5	-5	9.3207	-1.3207	-0.2190	-0.9061	-0.0046	-0.6562	0.9322	38.1539
	4	-4	9.3224	-1.3224	-0.2460	-0.9065	-0.0047	-0.6749	0.9393	38.3866
	3	-3	9.3242	-1.3242	-0.2752	-0.9079	-0.0047	-0.6968	0.9487	38.5153
	2	-2	9.3260	-1.3260	-0.3054	-0.9103	-0.0047	-0.7213	0.9602	38.4350
	1	-1	9.3279	-1.3279	-0.3380	-0.9144	-0.0048	-0.7503	0.9749	38.1934
TS		0	9.3298	-1.3298	-0.3723	-0.9202	-0.0048	-0.7844	0.9927	37.6792
	1	1	9.3318	-1.3318	-0.4042	-0.9268	-0.0049	-0.8198	1.0111	36.9465
	2	2	9.3338	-1.3338	-0.4354	-0.9354	-0.0049	-0.8601	1.0317	35.8395
	3	3	9.3358	-1.3358	-0.4651	-0.9462	-0.0050	-0.9062	1.0544	34.3833
	4	4	9.3375	-1.3375	-0.4921	-0.9581	-0.0051	-0.9570	1.0771	32.9067
F	5	5	9.3386	-1.3386	-0.5154	-0.9692	-0.0052	-1.0099	1.0977	31.6444
	6	6	9.3385	-1.3385	-0.5345	-0.9732	-0.0053	-1.0573	1.1103	30.7308
	7	7	9.3388	-1.3388	-0.5496	-0.9704	-0.0053	-1.0942	1.1153	30.1777
	8	8	9.3398	-1.3398	-0.5603	-0.9613	-0.0053	-1.1198	1.1127	29.8688
	9	9	9.3414	-1.3414	-0.5651	-0.9449	-0.0052	-1.1305	1.1010	29.9933
	10	10	9.3429	-1.3429	-0.5671	-0.9282	-0.0051	-1.1385	1.0877	30.1623
	product-Al	22	9.3561	-1.3561	-0.5447	-0.8164	-0.0052	-1.1725	0.9814	31.4156
	Product		9.0970	-1.0970	0.8444	-0.3056	-0.0007	-0.9657	0.8980	27.8300

Table 14: Values of the descriptors during the reaction between cyclohexanone and Lithium aluminium hydride. cont.

	Step	Point	$N(C)$	$q(C)$	$\mu(C)$ $\mu_x(C)$	$\mu_y(C)$	$\mu_Z(C)$	$Q(C)$	$\lvert\mu(C)\rvert$	$\lvert\mu(CO)\rvert$
	Reactant		4.9682	1.0318	0.0943	-0.0389	0.0007	-1.2367	0.1020	1.3159
	reactant-Al	-11	5.0318	0.9682	0.3137	0.0074	0.0036	-0.9839	0.3138	1.9804
	10	-10	5.0711	0.9289	0.5221	0.5948	0.0040	-0.7843	0.7914	0.5286
	9	-9	5.0737	0.9263	0.5123	0.5956	0.0040	-0.7783	0.7856	0.5021
	8	-8	5.0757	0.9243	0.5023	0.5954	0.0040	-0.7686	0.7789	0.4768
	7	-7	5.0786	0.9214	0.4911	0.5938	0.0039	-0.7584	0.7706	0.4510
	6	-6	5.0828	0.9172	0.4823	0.5917	0.0040	-0.7532	0.7634	0.4281
R	5	-5	5.0878	0.9122	0.4710	0.5899	0.0036	-0.7448	0.7549	0.4043
	4	-4	5.0926	0.9074	0.4585	0.5861	0.0032	-0.7314	0.7441	0.3845
	3	-3	5.0987	0.9013	0.4455	0.5781	0.0036	-0.7198	0.7298	0.3712
	2	-2	5.1048	0.8952	0.4284	0.5658	0.0031	-0.7020	0.7097	0.3658
	1	-1	5.1132	0.8868	0.4090	0.5505	0.0031	-0.6870	0.6858	0.3707
TS		0	5.1235	0.8765	0.3839	0.5310	0.0042	-0.6700	0.6553	0.3893
	1	1	5.1352	0.8648	0.3581	0.5095	0.0031	-0.6533	0.6227	0.4198
	2	2	5.1471	0.8529	0.3277	0.4796	0.0032	-0.6324	0.5808	0.4684
	3	3	5.1600	0.8400	0.2918	0.4418	0.0020	-0.6072	0.5294	0.5334
	4	4	5.1747	0.8253	0.2553	0.3996	0.0024	-0.5950	0.4742	0.6066
F	5	5	5.1889	0.8111	0.2165	0.3553	0.0024	-0.6095	0.4161	0.6828
	6	6	5.2023	0.7977	0.1874	0.3195	0.0030	-0.6242	0.3704	0.7402
	7	7	5.2115	0.7885	0.1657	0.2936	0.0023	-0.6389	0.3372	0.7781
	8	8	5.2171	0.7829	0.1490	0.2751	0.0024	-0.6484	0.3129	0.8000
	9	9	5.2182	0.7818	0.1421	0.2696	0.0023	-0.6550	0.3048	0.7968
	10	10	5.2185	0.7815	0.1362	0.2658	0.0025	-0.6596	0.2987	0.7902
	product-Al	22	5.2146	0.7854	0.1025	0.2296	0.0013	-0.6824	0.2514	0.7348
	Product		5.4511	0.5489	-0.0206	0.0374	0.0010	-0.5677	0.0427	0.8663

Table 15: Values of the descriptors during the reaction between cyclohexanone and Lithium aluminium hydride. cont.

	Step	Point	$N(H)$	$q(H)$	$\mu_x(H)$	$\mu(H)$ $\mu_y(H)$	$\mu_Z(H)$	$Q(H)$	$\lvert\mu(H)\rvert$
	Reactant		-	-	-	-	-	-	-
	reactant-Al	-11	1.8232	-0.8232	-0.0830	0.9522	0.0074	-0.9157	0.9559
	10	-10	1.7115	-0.7115	0.1298	0.3661	0.0034	-0.6483	0.3885
	9	-9	1.7048	-0.7048	0.1325	0.3669	0.0034	-0.6388	0.3901
	8	-8	1.6979	-0.6979	0.1354	0.3668	0.0032	-0.6310	0.3910
	7	-7	1.6897	-0.6897	0.1381	0.3655	0.0030	-0.6214	0.3907
	6	-6	1.6807	-0.6807	0.1405	0.3629	0.0029	-0.6120	0.3892
R	5	-5	1.6701	-0.6701	0.1432	0.3594	0.0028	-0.6012	0.3869
	4	-4	1.6582	-0.6582	0.1463	0.3553	0.0029	-0.5873	0.3843
	3	-3	1.6442	-0.6442	0.1483	0.3491	0.0028	-0.5731	0.3793
	2	-2	1.6283	-0.6283	0.1482	0.3406	0.0027	-0.5562	0.3715
	1	-1	1.6091	-0.6091	0.1462	0.3294	0.0026	-0.5390	0.3604
TS		0	1.5862	-0.5862	0.1410	0.3150	0.0023	-0.5128	0.3452
	1	1	1.5618	-0.5618	0.1330	0.2994	0.0023	-0.4872	0.3277
	2	2	1.5343	-0.5343	0.1229	0.2809	0.0018	-0.4595	0.3066
	3	3	1.5027	-0.5027	0.1101	0.2607	0.0019	-0.4251	0.2830
	4	4	1.4689	-0.4689	0.0952	0.2392	0.0017	-0.3902	0.2574
F	5	5	1.4356	-0.4356	0.0793	0.2178	0.0017	-0.3569	0.2318
	6	6	1.4096	-0.4096	0.0652	0.1996	0.0014	-0.3308	0.2099
	7	7	1.3914	-0.3914	0.0550	0.1864	0.0010	-0.3159	0.1943
	8	8	1.3789	-0.3789	0.0473	0.1773	0.0007	-0.3060	0.1835
	9	9	1.3752	-0.3752	0.0446	0.1755	0.0008	-0.3060	0.1811
	10	10	1.3735	-0.3735	0.0430	0.1754	0.0008	-0.3058	0.1806
	product-Al	22	1.3630	-0.3630	0.0218	0.1740	0.0013	-0.2904	0.1754
	Product		0.4454	-0.0216	0.1075	0.1093	0.0007	-0.1735	0.1533