

Table 1. The calculated quantum chemical parameters at B3LYP/631G(d,p)

Solvent	Molecule	HOMO (-I)	LUMO (-A)	ΔE	μ	η	W	ΔN_{max}
Gas	Basic	-0,21270	-0,04547	4,55056	-3,51258	2,27528	2,71137	1,54380
	A	-0,19593	-0,06598	3,53612	-3,56347	1,76806	3,59103	2,01547
	B	-0,20979	-0,04632	4,44825	-3,48456	2,22412	2,72964	1,56671
	C	-0,20733	-0,05280	4,20498	-3,53925	2,10249	2,97892	1,68336
	D	-0,19899	-0,04969	4,06266	-3,38347	2,03133	2,81782	1,66564
	E	-0,20962	-0,04737	4,41505	-3,49653	2,20752	2,76910	1,58391
Toluen	Basic	-0,21337	-0,04733	4,51818	-3,54701	2,25909	2,78458	1,57010
	A	-0,19699	-0,06701	3,53694	-3,59190	1,76847	3,64773	2,03108
	B	-0,21192	-0,04760	4,47138	-3,53095	2,23569	2,78832	1,57936
	C	-0,20903	-0,05407	4,21668	-3,57966	2,10834	3,03888	1,69786
	D	-0,20114	-0,05186	4,06212	-3,44224	2,03106	2,91696	1,69480
	E	-0,21157	-0,04922	4,41777	-3,54823	2,20889	2,84984	1,60634
Chloroform	Basic	-0,21396	-0,04866	4,49804	-3,57313	2,24902	2,83840	1,58875
	A	-0,19822	-0,06824	3,53694	-3,62537	1,76847	3,71602	2,05001
	B	-0,21312	-0,04928	4,45832	-3,57014	2,22916	2,85890	1,60156
	C	-0,21026	-0,05521	4,21913	-3,61191	2,10956	3,09208	1,71216
	D	-0,20265	-0,05341	4,06103	-3,48388	2,03051	2,98875	1,71576
	E	-0,21284	-0,05071	4,41178	-3,58578	2,20589	2,91443	1,62555
Chlorobenzene	Basic	-0,21409	-0,04896	4,49342	-3,57898	2,24671	2,85063	1,59299
	A	-0,19852	-0,06855	3,53667	-3,63367	1,76833	3,73334	2,05486
	B	-0,21337	-0,04966	4,45478	-3,57871	2,22739	2,87492	1,60668
	C	-0,21054	-0,05547	4,21967	-3,61925	2,10984	3,10427	1,71542
	D	-0,20299	-0,05375	4,06103	-3,49313	2,03051	3,00464	1,72032
	E	-0,21310	-0,05105	4,40961	-3,59395	2,20480	2,92916	1,63005
Dichloromethane	Basic	-0,21436	-0,04953	4,48526	-3,59041	2,24263	2,87409	1,60098
	A	-0,19914	-0,06916	3,53694	-3,65041	1,76847	3,76752	2,06416
	B	-0,21384	-0,05040	4,44743	-3,59517	2,22372	2,90623	1,61674
	C	-0,21109	-0,05594	4,22185	-3,63313	2,11092	3,12651	1,72111
	D	-0,20366	-0,05438	4,06212	-3,51081	2,03106	3,03433	1,72856
	E	-0,21360	-0,05173	4,40471	-3,61000	2,20235	2,95867	1,63915
Quinoline	Basic	-0,21437	-0,04956	4,48471	-3,59095	2,24236	2,87531	1,60142
	A	-0,19917	-0,06919	3,53694	-3,65123	1,76847	3,76921	2,06463
	B	-0,21386	-0,05043	4,44716	-3,59585	2,22358	2,90751	1,61714
	C	-0,21112	-0,05596	4,22212	-3,63381	2,11106	3,12748	1,72132
	D	-0,20369	-0,05441	4,06212	-3,51163	2,03106	3,03574	1,72897
	E	-0,21363	-0,05176	4,40471	-3,61082	2,20235	2,96001	1,63953
Ethanol	Basic	-0,21471	-0,05028	4,47437	-3,60537	2,23719	2,90515	1,61157
	A	-0,20001	-0,07003	3,53694	-3,67408	1,76847	3,81655	2,07755
	B	-0,21440	-0,05137	4,43627	-3,61599	2,21814	2,94737	1,63019
	C	-0,21180	-0,05656	4,22430	-3,65123	2,11215	3,15590	1,72868
	D	-0,20457	-0,05519	4,06484	-3,53422	2,03242	3,07286	1,73892
	E	-0,21424	-0,05264	4,39736	-3,63109	2,19868	2,99834	1,65149
Methanol	Basic	-0,21476	-0,05039	4,47274	-3,60755	2,23637	2,90972	1,61313
	A	-0,20014	-0,07016	3,53694	-3,67762	1,76847	3,82390	2,07955
	B	-0,21448	-0,05151	4,43464	-3,61898	2,21732	2,95334	1,63214
	C	-0,21191	-0,05664	4,22511	-3,65381	2,11256	3,15976	1,72957
	D	-0,20471	-0,05531	4,06538	-3,53775	2,03269	3,07860	1,74043
	E	-0,21433	-0,05277	4,39627	-3,63408	2,19814	3,00403	1,65326
Acetonitrile	Basic	-0,21477	-0,05043	4,47192	-3,60823	2,23596	2,91135	1,61373
	A	-0,20018	-0,0702	3,536937772	-3,679	1,768	3,826	2,080
	B	-0,2145	-0,05155	4,43409763	-3,620	2,217	2,955	1,633
	C	-0,21194	-0,05667	4,225114078	-3,655	2,113	3,161	1,730

	D	-0,20474	-0,05534	4,06538316	-3,539	2,033	3,080	1,741
	E	-0,21435	-0,0528	4,39600167	-3,635	2,198	3,005	1,654
DMSO	Basic	-0,21481	-0,05050	4,47111	-3,60973	2,23555	2,91430	1,61469
	A	-0,20028	-0,07029	3,53721	-3,68129	1,76860	3,83125	2,08147
	B	-0,21455	-0,05165	4,43274	-3,62184	2,21637	2,95928	1,63413
	C	-0,21202	-0,05673	4,22566	-3,65653	2,11283	3,16406	1,73063
	D	-0,20484	-0,05542	4,06593	-3,54102	2,03296	3,08388	1,74180
	E	-0,21442	-0,05290	4,39519	-3,63708	2,19759	3,00973	1,65503
Water	Basic	-0,21486	-0,05061	4,4694725	-3,612	2,235	2,919	1,616
	A	-0,2004	-0,07042	3,5369378	-3,685	1,768	3,839	2,084
	B	-0,21462	-0,05179	4,4308323	-3,625	2,215	2,965	1,636
	C	-0,21212	-0,05682	4,2259304	-3,659	2,113	3,168	1,732
	D	-0,20496	-0,05554	4,0659274	-3,544	2,033	3,090	1,743
	E	-0,2145	-0,05302	4,3940969	-3,640	2,197	3,015	1,657

Table 2. The calculated quantum chemical parameters at B3LYP/631+G(d,p)

Solvent	Molecule	HOMO (-I)	LUMO (-A)	ΔE	μ	η	W	ΔN_{max}
Gas	Basic	-0,22296	-0,05905	4,46022	-3,83694	2,23011	3,30076	1,72052
	A	-0,20607	-0,07800	3,48496	-3,86497	1,74248	4,28642	2,21808
	B	-0,22021	-0,05916	4,38240	-3,80102	2,19120	3,29678	1,73468
	C	-0,21767	-0,06501	4,15409	-3,84606	2,07705	3,56087	1,85170
	D	-0,20976	-0,06183	4,02538	-3,69517	2,01269	3,39205	1,83594
	E	-0,22034	-0,05967	4,37206	-3,80973	2,18603	3,31973	1,74276
Toluen	Basic	-0,22290	-0,06011	4,42974	-3,85055	2,21487	3,34708	1,73850
	A	-0,20623	-0,07812	3,48605	-3,86878	1,74303	4,29353	2,21958
	B	-0,22146	-0,06007	4,39165	-3,83041	2,19582	3,34090	1,74441
	C	-0,21886	-0,06519	4,18158	-3,86470	2,09079	3,57184	1,84844
	D	-0,21108	-0,06325	4,02266	-3,73245	2,01133	3,46318	1,85571
	E	-0,22147	-0,06088	4,36988	-3,84157	2,18494	3,37713	1,75820
Chloroform	Basic	-0,22325	-0,06120	4,40961	-3,87014	2,20480	3,39667	1,75532
	A	-0,20718	-0,07904	3,48687	-3,89422	1,74343	4,34917	2,23365
	B	-0,22243	-0,06156	4,37750	-3,86388	2,18875	3,41053	1,76534
	C	-0,22016	-0,06577	4,20117	-3,89028	2,10058	3,60239	1,85200
	D	-0,21287	-0,06429	4,04307	-3,77096	2,02153	3,51716	1,86539
	E	-0,22236	-0,06246	4,35110	-3,87518	2,17555	3,45131	1,78124
Chlorobenzene	Basic	-0,22334	-0,06147	4,40471	-3,87504	2,20235	3,40906	1,75950
	A	-0,20744	-0,07930	3,48687	-3,90130	1,74343	4,36498	2,23771
	B	-0,22265	-0,06193	4,37342	-3,87191	2,18671	3,42791	1,77066
	C	-0,22042	-0,06600	4,20198	-3,89694	2,10099	3,61405	1,85481
	D	-0,21322	-0,06460	4,04416	-3,77994	2,02208	3,53298	1,86933
	E	-0,22256	-0,06284	4,34620	-3,88307	2,17310	3,46928	1,78688
Dichloromethane	Basic	-0,22354	-0,06200	4,39573	-3,88497	2,19786	3,43356	1,76761
	A	-0,20799	-0,07984	3,48714	-3,91613	1,74357	4,39789	2,24604
	B	-0,22305	-0,06267	4,36416	-3,88742	2,18208	3,46276	1,78152
	C	-0,22088	-0,06649	4,20117	-3,90987	2,10058	3,63877	1,86133
	D	-0,21384	-0,06525	4,04334	-3,79721	2,02167	3,56607	1,87826
	E	-0,22295	-0,06358	4,33668	-3,89844	2,16834	3,50449	1,79789
Quinoline	Basic	-0,22355	-0,06202	4,39546	-3,88538	2,19773	3,43449	1,76791
	A	-0,20802	-0,07987	3,48714	-3,91694	1,74357	4,39972	2,24651
	B	-0,22307	-0,06270	4,36389	-3,88810	2,18195	3,46418	1,78194

	C	-0,22090	-0,06652	4,20090	-3,91055	2,10045	3,64027	1,86177
	D	-0,21387	-0,06528	4,04334	-3,79803	2,02167	3,56760	1,87866
	E	-0,22297	-0,06362	4,33614	-3,89926	2,16807	3,50640	1,79849
Ethanol	Basic	-0,22381	-0,06273	4,38321	-3,89858	2,19161	3,46753	1,77887
	A	-0,20880	-0,08064	3,48741	-3,93803	1,74371	4,44688	2,25843
	B	-0,22356	-0,06371	4,34974	-3,90851	2,17487	3,51203	1,79712
	C	-0,22145	-0,06723	4,19654	-3,92769	2,09827	3,67607	1,87187
	D	-0,21462	-0,06617	4,03953	-3,82034	2,01977	3,61305	1,89148
	E	-0,22347	-0,06460	4,32308	-3,91939	2,16154	3,55341	1,81324
Methanol	Basic	-0,22385	-0,06284	4,38131	-3,90062	2,19065	3,47267	1,78057
	A	-0,20892	-0,08077	3,48714	-3,94144	1,74357	4,45491	2,26055
	B	-0,22363	-0,06386	4,34757	-3,91150	2,17378	3,51918	1,79940
	C	-0,22153	-0,06734	4,19573	-3,93028	2,09786	3,68163	1,87347
	D	-0,21473	-0,06631	4,03872	-3,82375	2,01936	3,62022	1,89355
	E	-0,22354	-0,06476	4,32063	-3,92252	2,16031	3,56110	1,81572
Acetonitrile	Basic	-0,22386	-0,06287	4,38076	-3,90116	2,19038	3,47407	1,78104
	A	-0,20896	-0,08080	3,48741	-3,94239	1,74371	4,45672	2,26092
	B	-0,22365	-0,06391	4,34675	-3,91246	2,17337	3,52155	1,80018
	C	-0,22156	-0,06738	4,19545	-3,93123	2,09773	3,68365	1,87404
	D	-0,21476	-0,06635	4,03844	-3,82470	2,01922	3,62227	1,89414
	E	-0,22356	-0,06480	4,32008	-3,92334	2,16004	3,56303	1,81633
DMSO	Basic	-0,22389	-0,06295	4,37940	-3,90266	2,18970	3,47781	1,78228
	A	-0,20905	-0,08089	3,48741	-3,94484	1,74371	4,46226	2,26233
	B	-0,22370	-0,06402	4,34512	-3,91463	2,17256	3,52680	1,80185
	C	-0,22162	-0,06746	4,19491	-3,93314	2,09745	3,68770	1,87519
	D	-0,21484	-0,06645	4,03790	-3,82715	2,01895	3,62739	1,89561
	E	-0,22361	-0,06491	4,31845	-3,92552	2,15922	3,56834	1,81802
Water	Basic	-0,22393	-0,06306	4,37750	-3,90470	2,18875	3,48297	1,78399
	A	-0,20917	-0,08101	3,48741	-3,94810	1,74371	4,46965	2,26420
	B	-0,22377	-0,06417	4,34294	-3,91763	2,17147	3,53396	1,80414
	C	-0,22169	-0,06757	4,19382	-3,93558	2,09691	3,69325	1,87685
	D	-0,21494	-0,06659	4,03681	-3,83041	2,01841	3,63457	1,89774
	E	-0,22368	-0,06505	4,31654	-3,92837	2,15827	3,57511	1,82015

Table 3. The calculated quantum chemical parameters at B3LYP/ 6311++G(d,p)

Solvent	Molecule	HOMO (-I)	LUMO (-A)	ΔE	μ	η	W	ΔN_{max}
Gas	Basic	-0,22464	-0,06097	4,45369	-3,88592	2,22684	3,39054	1,74504
	A	-0,20813	-0,07967	3,49558	-3,91572	1,74779	4,38636	2,24039
	B	-0,22178	-0,06115	4,37097	-3,84946	2,18548	3,39018	1,76138
	C	-0,21947	-0,06667	4,15790	-3,89313	2,07895	3,64523	1,87264
	D	-0,21163	-0,06351	4,03055	-3,74347	2,01528	3,47684	1,85755
	E	-0,22192	-0,06168	4,36035	-3,85858	2,18018	3,41454	1,76985
Toluen	Basic	-0,22483	-0,06222	4,42485	-3,90552	2,21242	3,44714	1,76527
	A	-0,20854	-0,08002	3,49721	-3,92606	1,74860	4,40750	2,24525
	B	-0,22330	-0,06215	4,38512	-3,88375	2,19256	3,43970	1,77133
	C	-0,22074	-0,06725	4,17668	-3,91831	2,08834	3,67592	1,87628
	D	-0,21305	-0,06527	4,02130	-3,78674	2,01065	3,56586	1,88334
	E	-0,22332	-0,06297	4,36335	-3,89518	2,18167	3,47724	1,78541
Chloroform	Basic	-0,22529	-0,06335	4,40661	-3,92715	2,20331	3,49985	1,78239
	A	-0,20959	-0,08105	3,49775	-3,95436	1,74888	4,47057	2,26109
	B	-0,22440	-0,06359	4,37587	-3,91831	2,18793	3,50859	1,79087
	C	-0,22223	-0,06779	4,20253	-3,94593	2,10126	3,70499	1,87788
	D	-0,21488	-0,06636	4,04144	-3,82647	2,02072	3,62293	1,89362
	E	-0,22431	-0,06456	4,34702	-3,93028	2,17351	3,55349	1,80826

Chlorobenzene	Basic	-0,22540	-0,06362	4,40226	-3,93232	2,20113	3,51254	1,78650
	A	-0,20988	-0,08133	3,49803	-3,96212	1,74901	4,48778	2,26534
	B	-0,22464	-0,06395	4,37260	-3,92647	2,18630	3,52586	1,79594
	C	-0,22249	-0,06803	4,20307	-3,95273	2,10154	3,71729	1,88088
	D	-0,21533	-0,06664	4,04606	-3,83640	2,02303	3,63760	1,89636
	E	-0,22453	-0,06493	4,34294	-3,93831	2,17147	3,57137	1,81366
Dichloromethane	Basic	-0,22564	-0,06415	4,39437	-3,94280	2,19718	3,53763	1,79448
	A	-0,21046	-0,08190	3,49830	-3,97776	1,74915	4,52294	2,27411
	B	-0,22509	-0,06466	4,36552	-3,94225	2,18276	3,56002	1,80608
	C	-0,22298	-0,06855	4,20226	-3,96647	2,10113	3,74391	1,88778
	D	-0,21600	-0,06729	4,04661	-3,85436	2,02330	3,67124	1,90498
	E	-0,22496	-0,06565	4,33505	-3,95395	2,16752	3,60636	1,82418
Quinoline	Basic	-0,22565	-0,06418	4,39382	-3,94334	2,19691	3,53904	1,79495
	A	-0,21049	-0,08193	3,49830	-3,97858	1,74915	4,52480	2,27458
	B	-0,22512	-0,06470	4,36525	-3,94320	2,18263	3,56196	1,80663
	C	-0,22300	-0,06858	4,20198	-3,96715	2,10099	3,74544	1,88823
	D	-0,21603	-0,06732	4,04661	-3,85518	2,02330	3,67280	1,90539
	E	-0,22498	-0,06568	4,33478	-3,95463	2,16739	3,60783	1,82461
Ethanol	Basic	-0,22596	-0,06487	4,38348	-3,95695	2,19174	3,57191	1,80539
	A	-0,21131	-0,08274	3,49857	-4,00076	1,74928	4,57503	2,28708
	B	-0,22565	-0,06564	4,35410	-3,96320	2,17705	3,60741	1,82045
	C	-0,22359	-0,06930	4,19845	-3,98497	2,09922	3,78235	1,89831
	D	-0,21682	-0,06822	4,04361	-3,87817	2,02181	3,71949	1,91817
	E	-0,22552	-0,06662	4,32389	-3,97477	2,16195	3,65384	1,83851
Methanol	Basic	-0,22600	-0,06497	4,38185	-3,95885	2,19093	3,57668	1,80693
	A	-0,21144	-0,08287	3,49857	-4,00429	1,74928	4,58312	2,28910
	B	-0,22573	-0,06579	4,35219	-3,96633	2,17610	3,61469	1,82268
	C	-0,22368	-0,06942	4,19763	-3,98783	2,09882	3,78852	1,90004
	D	-0,21694	-0,06836	4,04307	-3,88171	2,02153	3,72678	1,92018
	E	-0,22561	-0,06677	4,32226	-3,97803	2,16113	3,66122	1,84072
Acetonitrile	Basic	-0,22602	-0,06500	4,38158	-3,95953	2,19079	3,57814	1,80735
	A	-0,21148	-0,08291	3,49857	-4,00538	1,74928	4,58561	2,28973
	B	-0,22575	-0,06583	4,35165	-3,96715	2,17582	3,61663	1,82329
	C	-0,22371	-0,06945	4,19763	-3,98865	2,09882	3,79007	1,90043
	D	-0,21697	-0,06840	4,04280	-3,88266	2,02140	3,72886	1,92078
	E	-0,22563	-0,06681	4,32171	-3,97885	2,16086	3,66319	1,84133
DMSO	Basic	-0,22605	-0,06508	4,38022	-3,96103	2,19011	3,58195	1,80860
	A	-0,21158	-0,08300	3,49884	-4,00797	1,74942	4,59118	2,29103
	B	-0,22581	-0,06594	4,35029	-3,96946	2,17514	3,62198	1,82492
	C	-0,22377	-0,06953	4,19709	-3,99055	2,09854	3,79418	1,90158
	D	-0,21705	-0,06850	4,04225	-3,88511	2,02113	3,73407	1,92225
	E	-0,22569	-0,06692	4,32035	-3,98116	2,16018	3,66860	1,84298
Water	Basic	-0,22610	-0,06518	4,37886	-3,96307	2,18943	3,58676	1,81009
	A	-0,21171	-0,08313	3,49884	-4,01150	1,74942	4,59928	2,29305
	B	-0,22588	-0,06608	4,34838	-3,97232	2,17419	3,62878	1,82703
	C	-0,22385	-0,06964	4,19627	-3,99314	2,09813	3,79984	1,90318
	D	-0,21716	-0,06863	4,04171	-3,88837	2,02085	3,74085	1,92412
	E	-0,22576	-0,06705	4,31872	-3,98389	2,15936	3,67501	1,84494