Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information to the manuscript "The effect of N-heterocyclic carbene units on the absorption spectra of Fe(II) complexes: a challenge for theory"

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1 Reoptimised geometries for TDDFT

1.1 IC1 geometry

Table 1: XYZ coordinates of the optimised geometry of IC1

Atom	x	y	z	Atom	x	y	z
C	0.81129200	2.07011900	0.98199900	H	-5.59938800	2.71583900	0.08658200
C	-0.76886500	2.03631800	-0.74852400	C	-5.55453800	0.36269400	1.34513000
C	0.81995400	3.45881200	0.98956600	H	-6.12720100	-0.09482000	0.53549600
C	-0.80107900	3.42377100	-0.78900800	H	-5.28506100	-0.42277500	2.04971300
C	0.00383900	4.13360600	0.09205900	H	-6.20428100	1.07433500	1.86045900
H	1.44821800	4.00507100	1.67852600	C	-0.91870800	0.86594200	4.59319100
H	-1.43786300	3.94415200	-1.49029400	H	-0.41293300	0.12194100	3.97015700
H	-0.00513100	5.21463400	0.07900100	C	-1.66376600	0.12124700	5.71066000
Fe	0.04560100	-0.48699800	0.14554900	H	-0.94978900	-0.41547000	6.33910800
N	0.02727800	1.40103700	0.12445700	H	-2.20090200	0.83438400	6.34083900
C	-0.88402600	-4.48603900	0.92513900	H	-2.38201500	-0.60203000	5.32842300
C	-0.82375100	-3.10456100	0.90586300	C	0.14783900	1.75364300	5.23589500
C	0.88695300	-3.10640200	-0.64079500	H	0.61938800	2.42265600	4.51627000
C	0.91117400	-4.48810200	-0.69604000	H	-0.27805200	2.36411400	6.03535400
C	0.00585900	-5.17073200	0.10691600	H	0.92438600	1.12977800	5.68145500
H	-1.59259000	-5.01105700	1.54773700	C	4.56478600	0.89331300	-0.42983700
H	1.60226800	-5.01531000	-1.33615800	H	3.90697000	0.14465200	0.02199900
H	-0.00807800	-6.25168100	0.09283600	C	5.09599200	1.79518100	0.68520000
N	0.04336100	-2.43708900	0.14474400	H	5.92187000	2.41550900	0.32988300
C	1.52588400	-0.87650800	-1.18971000	H	4.32747100	2.45553900	1.08663900
C	2.69406800	-2.52901200	-2.27443300	H	5.47845700	1.18126800	1.50231300
C	3.16854100	-1.34153700	-2.68439100	C	5.75455100	0.15850800	-1.06425400
H	2.97263300	-3.53082600	-2.54562300	H	5.44826100	-0.57288400	-1.81016400
H	3.94439700	-1.10591200	-3.38918000	H	6.42307500	0.87647400	-1.54573100
C	-1.42278300	-0.87377600	1.49356400	H	6.32095700	-0.36692400	-0.29232400
C	-2.62448700	-2.52365700	2.54510800	C	1.04921400	1.05329500	-4.15598800
C	-3.06903800	-1.33536300	2.98523100	H	0.50967400	0.31725200	-3.55267200
H	-2.92729300	-3.52490200	2.79138100	C	1.72725800	0.30700700	-5.31398100
H	-3.84098700	-1.09812700	3.69366800	H	0.97094700	-0.15930400	-5.94903400
N	-1.62083700	-2.22924800	1.63870000	H	2.29986400	1.00756700	-5.92678500
N	-2.33001800	-0.34058900	2.34330200	H	2.40295000	-0.47471800	-4.97008600
N	1.69533300	-2.23261700	-1.36320400	C	0.02789100	2.02990300	-4.73890000
N	2.45435300	-0.34509300	-2.01735600	H	-0.78775200	1.47398800	-5.20377900
C	-2.55962600	1.05785200	2.62888000	H	-0.39605300	2.68807300	-3.97959400
C	-3.52232800	1.74940100	1.87774900	H	0.47800600	2.65624500	-5.51228100
C	-1.88414600	1.64067300	3.71312900	C	-1.53406900	1.10582500	-1.58207400
C	-3.76527800	3.07949500	2.21510700	C	-2.43655400	1.48952200	-2.56328300
C	-2.16949100	2.97333200	4.00400600	C	-1.93624400	-1.13170400	-2.02308100
C	-3.09535500	3.68703000	3.26292800	C	-3.10310300	0.51897000	-3.29119000
H	-4.49270600	3.64750700	1.65198700	H	-2.61640000	2.53781500	-2.75509200
H	-1.66146800	3.45914000	4.82553400	C	-2.84784500	-0.81546800	-3.01633500
H	-3.30006800	4.72190800	3.50685700	H	-1.71494300	-2.16322400	-1.78467500
C	2.74841200	1.05340900	-2.23585700	H	-3.80954900	0.80127300	-4.05976300
C	2.07658600	1.73015000	-3.26585400	H	-3.34316200	-1.60866400	-3.55785800
C	3.76726800	1.65096900	-1.47702500	C	1.59198800	1.17135000	1.83651000
C	2.42478900	3.06024500	-3.49273700	C	2.48649700	1.59092300	2.80968100
C	4.07349500	2.98268300	-1.75097300	C	2.03471700	-1.05008100	2.32261200
C	3.40892400	3.68176600	-2.74350600	C	3.17060100	0.64704100	3.55681200
H	1.92151800	3.61717300	-4.27081200	H	2.64546000	2.64641200	2.98061500
H	4.84582900	3.47931000	-1.18006100	C	2.94052200	-0.69700100	3.30920300
H	3.66288500	4.71619900	-2.93798100	H	1.83069400	-2.08944500	2.10282700
C	-4.32826100	1.08855200	0.77362400	H	3.87144000	0.95775100	4.31955300
H	-3.69193200	0.34211700	0.28903400	H	3.45057600	-1.46960500	3.86663200
C	-4.79975800	2.07621500	-0.29350300	N	1.37124700	-0.14649700	1.59766700
H	-3.99362500	2.72145900	-0.64464300	N	-1.28874500	-0.20230800	-1.31586000
H	-5.19882900	1.52998500	-1.14949900				

1.2 IC2 geometry

Table 2: XYZ coordinates of the optimised geometry of IC2

Atom	x	y	z	Atom	x	y	z
C	0.576129	2.511719	0.990420	N	-2.373520	-0.064844	2.259140
C	-1.035981	2.516132	-0.667559	N	1.527778	-1.692786	-1.592695
C	0.546318	3.890589	1.098114	N	2.098801	0.282506	-2.183241
C	-1.140710	3.895138	-0.637639	C	-2.409202	-1.729797	-2.475335
C	-0.329835	4.574822	0.263785	H	-1.705442	-2.180394	-1.779557
H	1.177160	4.412727	1.802198	C	-3.808945	-2.228119	-2.153117
H	-1.825101	4.421100	-1.286696	H	-4.551865	-1.787215	-2.821503
H	-0.382626	5.653475	0.317925	H	-3.847183	-3.310954	-2.277523
C	2.302001	1.866143	2.707628	H	-4.080016	-1.987870	-1.123508
C	1.227028	0.281280	1.449231	C	2.346489	-1.739973	2.393907
H	2.554414	2.849230	3.061634	H	1.668418	-2.188752	1.672052
C	2.762933	0.653692	3.065786	C	3.777512	-2.061723	1.993605
H	3.501494	0.385682	3.800119	H	3.988716	-1.702224	0.984850
C	-1.488051	0.287554	-1.330453	H	4.493468	-1.607771	2.682369
C	-2.705085	1.878369	-2.443931	H	3.928588	-3.141552	2.015584
H	-3.046379	2.862961	-2.707722	C	1.991655	-2.244005	3.783683
C	-3.055592	0.667248	-2.914566	H	0.956523	-2.002886	4.032071
H	-3.769406	0.402639	-3.674206	H	2.113203	-3.327234	3.819911
N	1.362156	1.629236	1.717016	H	2.643599	-1.807687	4.543733
N	2.099411	-0.294475	2.291864	C	-1.976413	-2.054503	-3.896221
N	-1.744044	1.637029	-1.474778	H	-0.963141	-1.695273	-4.085587
N	-2.307223	-0.284351	-2.227421	H	-1.994905	-3.134646	-4.045426
Fe	-0.115011	-0.090062	0.043412	H	-2.648737	-1.602258	-4.628673
N	-0.196382	1.846322	0.126953	C	-2.610251	1.368259	2.486898
C	-0.816046	-4.141487	0.743091	H	-1.915652	1.873417	1.820118
C	-0.833750	-2.758320	0.754504	C	-4.030689	1.741543	2.093940
C	0.808614	-2.632668	-0.868472	H	-4.229544	1.473366	1.054749
C	0.904018	-4.010039	-0.954841	H	-4.763739	1.240774	2.730250
C	0.072440	-4.758389	-0.129684	H	-4.168753	2.817563	2.206032
H	-1.465680	-4.716314	1.386705	C	-2.275109	1.741076	3.922265
H	1.596064	-4.484119	-1.634808	H	-1.245329	1.471580	4.163561
H	0.117489	-5.838084	-0.167826	H	-2.391369	2.817266	4.055388
N	-0.038873	-2.027261	-0.031658	H	-2.941491	1.241766	4.629160
C	1.276507	-0.359419	-1.337506	C	2.173630	1.743652	-2.330745
C	2.481186	-1.856381	-2.585033	H	1.637372	2.137030	-1.469683
C	2.835139	-0.611799	-2.955207	C	3.615284	2.220058	-2.267820
H	2.818443	-2.816514	-2.931390	H	4.103226	1.874938	-1.355186
H	3.545717	-0.288883	-3.694716	H	4.191772	1.870175	-3.126608
C	-1.485175	-0.571316	1.388717	H	3.633816	3.310214	-2.279089
C	-2.595137	-2.252120	2.480761	C	1.467616	2.180645	-3.605544
C	-3.058935	-1.072448	2.932497	H	0.431065	1.837494	-3.618166
H	-2.859465	-3.260995	2.740885	H	1.472789	3.269242	-3.674520
H	-3.813258	-0.865366	3.670338	H	1.973982	1.781755	-4.487575
N	-1.631910	-1.936150	1.536124				

1.3 IC3 geometry

Table 3: XYZ coordinates of the optimised geometry of IC3

Atom	x	y	z	Atom	x	y	z
Fe	0.000059848	-0.5468894843	0.0966273128	H	-1.636607945	3.3507625105	4.8628810729
N	-1.3491716787	-0.1836802874	-1.3769017669	C	-3.0707149483	3.6216592885	3.3080396509
N	-0.0025488241	1.3670673057	0.0930023749	H	-3.2643210289	4.6538777191	3.5712690208
N	1.4994361025	1.1193654278	1.7408233186	C	-3.7501692153	3.039333233	2.2518051431
N	2.0858637509	-0.8327056279	2.4018188645	H	-4.474472051	3.6242885138	1.7024428703
C	-2.0152951412	-1.0855294703	-2.102330781	C	-3.5215698054	1.7128557	1.8896605805
H	-1.8156425632	-2.1258832432	-1.8832444003	C	-0.9207510465	0.7547550307	4.5856897076
C	-2.9199485502	-0.7328916661	-3.090384491	H	-0.4229266058	0.0156794702	3.9506956134
H	-3.4308984193	-1.5052634917	-3.6472386009	C	-1.6729451219	-0.0004762017	5.6923630774
C	-3.1479103498	0.6118675985	-3.3398289621	H	-0.9639982485	-0.5539921648	6.3117651802
H	-3.8478175802	0.9231524239	-4.1030808154	H	-2.2026725824	0.7075227647	6.3343531567
C	-2.4626828714	1.5547084996	-2.5927617834	H	-2.3983930515	-0.7105323638	5.2995576211
H	-2.6216843762	2.6096579252	-2.764677228	C	0.1561014263	1.6211393244	5.2422526073
C	-1.5684529541	1.1333061117	-1.6181740316	H	0.6367493483	2.2935530112	4.5322433819
C	-0.7866378739	2.035674823	-0.767996287	H	-0.2634850242	2.2254150105	6.0496577452
C	-0.7911783615	3.4238593412	-0.780684059	H	0.9253778346	0.9824882093	5.6784558097
H	-1.4170326736	3.9720986831	-1.4695583238	C	-4.3421705277	1.0800200376	0.7787466082
C	0.0295927581	4.1002308776	0.114599549	H	-3.7179839793	0.3340485226	0.2788504349
H	0.0415084011	5.1812378741	0.1215616901	C	-4.8073536944	2.0906492954	-0.2707712313
C	0.8366169247	3.4005416268	1.0025335174	H	-3.9951162019	2.7306841268	-0.6165281177
H	1.4790832111	3.9124372308	1.704062893	H	-5.2175622843	1.5625407109	-1.1327012931
C	0.7836127558	2.0181910333	0.9514465797	H	-5.5970253157	2.7340932522	0.1230908916
C	2.416697801	1.3222536796	2.7609666024	C	-5.575363167	0.3597293205	1.3449405974
H	2.725271653	2.2950836931	3.096518545	H	-6.1574432608	-0.0772931946	0.5307673214
C	2.7810226897	0.0935569039	3.1737401706	H	-5.3121757463	-0.4405855878	2.0347771192
H	3.4701462921	-0.2088765763	3.9417727441	H	-6.2140448371	1.0703009441	1.875154485
C	1.287311007	-0.2236049846	1.5111810601	C	2.728436658	1.0079017715	-2.2430460067
C	2.1937985973	-2.2739411374	2.5709224183	C	2.0877809906	1.7219747096	-3.2685637941
H	2.4113904492	-2.7478276914	1.6162374509	C	2.4722706367	3.0473840184	-3.4652512131
H	1.2688855693	-2.6792514785	2.9800679845	H	1.9937669806	3.6312122084	-4.2390900041
N	-2.3496377249	-0.3985678831	2.3125719429	C	3.4611642181	3.6297219849	-2.6912216017
N	-1.6885325689	-2.2870440502	1.5564786347	H	3.7435555275	4.6608921882	-2.8620568104
N	-0.0470004064	-2.4893714231	0.040765996	C	4.0948918864	2.8948224244	-1.7038293674
N	1.5952073194	-2.2809857882	-1.4735621167	H	4.8718185111	3.36130104	-1.1144635628
N	2.4009756807	-0.3889268351	-2.0619895496	C	3.7528564164	1.5655722634	-1.460097995
C	-1.4616301095	-0.9317164031	1.4389735787	C	1.0550385526	1.0909459547	-4.1871679981
C	-3.1015109084	-1.3936820065	2.9411632805	H	0.50463397	0.3394561977	-3.6139789998
H	-3.8612577799	-1.1568737336	3.6625340635	C	1.7280517188	0.3807723542	-5.3716840685
C	-2.687616166	-2.5806038446	2.4695430992	H	0.968244123	-0.0521958287	-6.0258163737
H	-3.0093259956	-3.5804564787	2.6960317998	H	2.3107167007	1.0968053714	-5.9562775192
C	-0.9215007504	-3.1596193631	0.7918007014	H	2.3934463231	-0.4212667097	-5.0560713536
C	-1.0098331769	-4.5403115756	0.7771699602	C	0.0465898833	2.1019543613	-4.7359780279
H	-1.7219496429	-5.0656919762	1.395264428	H	-0.7761469835	1.5738759021	-5.2202178847
C	-0.144249298	-5.2228412733	-0.0688416836	H	-0.368818175	2.7382598398	-3.9540089752
H	-0.1807917159	-6.3024477245	-0.1102603704	H	0.5049398177	2.749252824	-5.4867497484
C	0.7653487256	-4.5374729602	-0.8653211812	C	4.5199610979	0.7669808635	-0.4189805681
H	1.437872853	-5.0618522838	-1.5270203496	H	3.8338087879	0.0380400312	0.0224716645
C	0.7716726518	-3.1568231092	-0.773629843	C	5.0794400397	1.6361767313	0.7090556782
C	2.5852014068	-2.5690174853	-2.3983395773	H	5.9254747683	2.2340055669	0.3626975275
H	2.8379268802	-3.5667029563	-2.7067964884	H	4.332340894	2.3153127265	1.1191266549
C	3.0882997075	-1.3799665832	-2.7663585195	H	5.439214144	0.9994064673	1.5183711469
H	3.8696010036	-1.1387384003	-3.4629673152	C	5.6850475936	-0.0044931893	-1.0576248391
C	1.4601744056	-0.9266520471	-1.2488464055	H	5.3546809966	-0.7189055224	-1.8095179869
C	-2.5617076707	0.9976545895	2.6240059296	H	6.3798835493	0.6927939792	-1.5320123952
C	-1.8788748134	1.5544508657	3.718198199	H	6.2307383077	-0.5558145012	-0.288911742
C	-2.1504095193	2.8849809659	4.0336583665	H	3.0070871642	-2.482773669	3.2604749833

1.4 IC4 geometry

Table 4: XYZ coordinates of the optimised geometry of IC4

Atom	x	y	z	Atom	x	y	z
C	5.281006	3.099312	-4.250013	N	4.324304	5.207074	0.031113
C	6.328195	2.233535	-3.958504	C	4.167776	7.061056	1.541179
C	6.511647	1.752461	-2.668976	C	5.347205	7.583917	1.038254
C	5.611304	2.169069	-1.704759	H	7.009413	1.931390	-4.742004
N	4.599905	2.993112	-1.983190	H	5.140874	3.473487	-5.253620
C	4.421233	3.468586	-3.226042	H	3.404258	4.848834	-5.396201
C	3.259074	4.357932	-3.314015	H	1.402035	6.316923	-5.340868
N	5.600032	1.813939	-0.358535	H	0.182396	6.600834	-3.173166
C	6.428118	0.973251	0.367823	H	1.014196	5.409596	-1.171386
C	5.946684	0.991146	1.625764	H	5.947988	5.162033	-1.235129
N	4.844790	1.839005	1.642345	H	6.927179	7.272029	-0.396775
C	4.606839	2.354439	0.428018	H	5.745779	8.509441	1.431000
C	1.736080	5.811916	-4.444708	H	3.630442	7.569682	2.329192
C	2.852449	4.993259	-4.477928	H	1.777034	6.563173	3.017584
N	2.593836	4.515857	-2.144000	H	-0.227569	5.201895	3.525207
C	1.520073	5.307258	-2.122704	H	-0.669817	3.114629	2.252656
C	1.058265	5.971889	-3.246357	H	-0.725770	1.131152	0.804599
Fe	3.398304	3.505961	-0.577876	C	2.570607	0.312141	-2.338670
C	2.444366	5.223503	1.471377	H	7.323134	1.081773	-2.426473
N	2.195725	4.087922	0.799659	C	4.031327	2.081512	2.823056
C	1.110802	3.358491	1.065988	H	3.733809	3.126460	2.854472
C	0.202197	3.717716	2.045532	H	4.621114	1.855987	3.708047
C	0.457745	4.886385	2.750585	H	3.144772	1.447199	2.812389
C	1.581527	5.653440	2.468830	N	1.766038	0.935218	-1.300028
N	1.058593	2.236305	0.243196	H	0.192904	-0.541200	-1.175759
C	3.678946	5.872460	1.019688	H	2.937127	1.071153	-3.025134
C	2.074788	2.079152	-0.673143	H	1.949477	-0.390503	-2.888240
C	0.596788	0.379430	-0.793243	H	3.412274	-0.223173	-1.898769
C	0.145071	1.196236	0.178015	H	6.288040	0.484933	2.511308
C	6.004216	6.901758	0.026442	H	7.267569	0.455007	-0.058858
C	5.459418	5.719910	-0.446886				

1.5 IC5 geometry

Table 5: XYZ coordinates of the optimised geometry of IC5

Atom	x	y	z	Atom	x	y	z
C	5.055727	2.920647	-4.311766	C	0.023560	0.115430	-0.417520
C	6.122181	2.066769	-4.064082	C	0.059073	1.198176	0.446339
C	6.385311	1.629164	-2.772925	C	6.138011	6.767241	-0.114562
C	5.559640	2.064025	-1.744690	C	5.532851	5.607333	-0.570384
N	4.534544	2.888795	-2.002533	N	4.416914	5.117293	-0.027365
C	4.266345	3.322247	-3.242650	C	4.406402	6.947340	1.518524
C	3.100870	4.213698	-3.282290	C	5.565144	7.448344	0.947417
C	5.658656	1.726030	-0.319493	H	6.751122	1.741083	-4.881017
C	6.627801	0.893816	0.218987	H	4.846765	3.262876	-5.314991
C	6.624970	0.647202	1.582529	H	7.215089	0.965874	-2.576057
C	5.651325	1.240915	2.369474	H	7.374580	0.444907	-0.420258
C	4.711899	2.061301	1.766432	H	7.372871	0.001198	2.021479
N	4.706094	2.304549	0.454607	H	5.610781	1.077648	3.436832
C	1.500117	5.629573	-4.353541	H	3.938313	2.540518	2.351452
C	2.609934	4.804019	-4.436524	H	3.091085	4.620465	-5.386743
N	2.523119	4.424119	-2.072700	H	1.101832	6.099403	-5.242379
C	1.455122	5.220774	-2.003040	H	0.046158	6.477004	-3.004384
C	0.912725	5.841334	-3.116545	H	1.022121	5.364789	-1.022227
Fe	3.425052	3.460334	-0.564501	H	5.953610	5.050958	-1.397104
C	2.630950	5.155406	1.532198	H	7.041236	7.120978	-0.590655
N	2.312269	4.033703	0.870484	H	6.011996	8.356676	1.327789
C	1.230889	3.306408	1.185471	H	3.935944	7.456333	2.347620
C	0.397156	3.702840	2.222493	H	2.083971	6.503548	3.120303
C	0.711264	4.861824	2.919327	H	0.076929	5.189910	3.731083
C	1.835934	5.601665	2.579489	H	-0.476936	3.124033	2.483441
C	1.085468	2.122731	0.329481	H	-0.701121	1.323973	1.204304
C	3.852930	5.781333	1.012905	H	-0.768538	-0.616885	-0.342069
N	2.056935	1.995023	-0.609351	H	1.029744	-0.839312	-2.069073
C	2.013856	0.948971	-1.436590	H	2.804237	0.879369	-2.171913
C	1.017190	-0.011335	-1.374842				

2 Excitation Energies

2.1 IC1 excited states

Table 6: Excited states of IC1

State	E [eV]	f	State	E [eV]
S1	2.5113	0.0061	T1	1.6824
S2	2.5392	0.0000	T2	1.7008
S3	2.6019	0.0013	T3	1.9631
S4	2.7590	0.0000	T4	2.1407
S5	2.7949	0.0126	T5	2.2201
S6	2.8486	0.0076	T6	2.2946
S7	2.8933	0.0003	T7	2.3343
S8	2.9137	0.0339	T8	2.4124
S9	2.9790	0.0001	T9	2.5826
S10	3.0099	0.0724	T10	2.6648
S11	3.0639	0.0011	T11	2.7464
S12	3.3378	0.0053	T12	2.7494
S13	3.3962	0.0024	T13	2.7680
S14	3.4754	0.0005	T14	2.9287
S15	3.6904	0.0000	T15	3.0497
S16	3.7499	0.0059	T16	3.1312
S17	3.7688	0.0832	T17	3.2242
S18	3.8158	0.0026	T18	3.3746
S19	3.8405	0.0070	T19	3.4568
S20	3.9166	0.0450	T20	3.5366
S21	3.9331	0.0307	T21	3.5508
S22	3.9489	0.0076	T22	3.6951
S23	3.9792	0.0002	T23	3.7319
S24	4.0026	0.0002	T24	3.7323
S25	4.0157	0.0083	T25	3.7942
S26	4.0589	0.0008	T26	3.8198
S27	4.0703	0.0002	T27	3.8532
S28	4.1149	0.0000	T28	3.9381
S29	4.1661	0.1950	T29	3.9560
S30	4.2572	0.0001	T30	3.9880
S31	4.2736	0.0009	T31	3.9983
S32	4.3114	0.0711	T32	4.0431
S33	4.3311	0.0053	T33	4.0818
S34	4.3491	0.0000	T34	4.0869
S35	4.3528	0.0000	T35	4.1051
S36	4.3860	0.0827	T36	4.1061
S37	4.4419	0.0595	T37	4.1198
S38	4.4983	0.0457	T38	4.1904
S39	4.5155	0.0008	T39	4.2213
S40	4.5558	0.0423	T40	4.2423
S41	4.5943	0.0265	T41	4.2662
S42	4.6169	0.0040	T42	4.2676
S43	4.6270	0.0002	T43	4.3083
S44	4.7387	0.0016	T44	4.3250
S45	4.7566	0.0485	T45	4.3284
S46	4.7903	0.0041	T46	4.3377
S47	4.8060	0.0014	T47	4.3877
S48	4.8153	0.0470	T48	4.4497
S49	4.8320	0.0010	T49	4.4650
S50	4.8494	0.0298	T50	4.4827

2.2 IC2 excited states

Table 7: Excited states of IC2

State	E [eV]	f	State	E [eV]
S1	2.8612	0.0022	T1	2.1330
S2	2.8687	0.0019	T2	2.1392
S3	2.9601	0.0002	T3	2.3597
S4	2.9663	0.0002	T4	2.6036
S5	3.1209	0.0000	T5	2.7156
S6	3.1563	0.0000	T6	2.7235
S7	3.2619	0.0000	T7	2.7364
S8	3.3342	0.0945	T8	2.8242
S9	3.4871	0.0020	T9	2.8478
S10	3.5003	0.0149	T10	3.0285
S11	3.5041	0.0141	T11	3.0665
S12	3.5526	0.1801	T12	3.0713
S13	3.7173	0.0000	T13	3.1500
S14	3.7945	0.0029	T14	3.2421
S15	3.8008	0.0030	T15	3.3115
S16	3.8830	0.0000	T16	3.3153
S17	4.2507	0.0048	T17	3.7146
S18	4.2534	0.0053	T18	3.7181
S19	4.4495	0.0571	T19	3.7901
S20	4.4568	0.0610	T20	3.8795
S21	4.6276	0.0468	T21	3.8808
S22	4.7024	0.0001	T22	3.9606
S23	4.7857	0.0000	T23	4.0648
S24	4.8144	0.0004	T24	4.0673
S25	4.8586	0.0150	T25	4.1414
S26	4.8624	0.0115	T26	4.1712
S27	4.8836	0.0646	T27	4.3280
S28	4.8850	0.0585	T28	4.5431
S29	4.9080	0.2266	T29	4.6310
S30	4.9774	0.0001	T30	4.6333
S31	5.0647	0.1040	T31	4.7131
S32	5.0692	0.1103	T32	4.7185
S33	5.0953	0.0066	T33	4.7682
S34	5.0977	0.0056	T34	4.7762
S35	5.1794	0.0003	T35	4.7769
S36	5.1840	0.0018	T36	4.8256
S37	5.1862	0.0013	T37	4.8500
S38	5.1936	0.0016	T38	4.8929
S39	5.1947	0.0195	T39	4.8978
S40	5.1988	0.0179	T40	4.9570
S41	5.2036	0.0198	T41	4.9595
S42	5.2274	0.0052	T42	4.9753
S43	5.2334	0.0730	T43	5.1251
S44	5.2384	0.0715	T44	5.1265
S45	5.3337	0.0001	T45	5.1313
S46	5.3761	0.0602	T46	5.1405
S47	5.3806	0.0606	T47	5.1561
S48	5.4019	0.3149	T48	5.1892
S49	5.4936	0.0654	T49	5.1904
S50	5.5525	0.0002	T50	5.2005

2.3 IC3 excited states

Table 8: Excited states of IC3

State	E [eV]	f	State	E [eV]
S1	2.5182	0.0103	T1	1.9586
S2	2.6430	0.0065	T2	2.0376
S3	2.7606	0.0010	T3	2.1145
S4	2.7811	0.0110	T4	2.2745
S5	2.8392	0.0448	T5	2.3082
S6	2.8687	0.0003	T6	2.3866
S7	2.9583	0.0000	T7	2.4286
S8	3.1194	0.0000	T8	2.4483
S9	3.2160	0.0079	T9	2.6839
S10	3.3118	0.0020	T10	2.8062
S11	3.3814	0.0090	T11	2.8161
S12	3.4267	0.0614	T12	2.8501
S13	3.5573	0.0347	T13	3.0605
S14	3.6056	0.0068	T14	3.1027
S15	3.6940	0.0405	T15	3.1278
S16	3.7251	0.0007	T16	3.2532
S17	3.8220	0.0151	T17	3.2906
S18	3.8614	0.0376	T18	3.4684
S19	3.8824	0.0002	T19	3.5304
S20	3.8992	0.0097	T20	3.5582
S21	3.9810	0.0006	T21	3.7276
S22	4.0152	0.0012	T22	3.7284
S23	4.0182	0.0010	T23	3.7492
S24	4.0653	0.0042	T24	3.7826
S25	4.2392	0.0020	T25	3.8582
S26	4.2535	0.0368	T26	3.9009
S27	4.2560	0.0008	T27	3.9276
S28	4.2938	0.0001	T28	3.9431
S29	4.3194	0.2056	T29	3.9808
S30	4.4879	0.0278	T30	3.9963
S31	4.5464	0.0481	T31	4.0685
S32	4.5516	0.0047	T32	4.0848
S33	4.5767	0.0151	T33	4.1102
S34	4.6009	0.0077	T34	4.1580
S35	4.6197	0.0013	T35	4.2024
S36	4.6230	0.0000	T36	4.2456
S37	4.6488	0.0001	T37	4.2696
S38	4.6769	0.0014	T38	4.2911
S39	4.6927	0.0228	T39	4.3328
S40	4.7292	0.1265	T40	4.4246
S41	4.7557	0.0800	T41	4.4365
S42	4.7570	0.0139	T42	4.4405
S43	4.8060	0.0060	T43	4.4463
S44	4.8065	0.0042	T44	4.5177
S45	4.8094	0.0005	T45	4.5307
S46	4.8349	0.0013	T46	4.5452
S47	4.8455	0.0113	T47	4.5714
S48	4.8614	0.0000	T48	4.5751
S49	4.8722	0.0232	T49	4.5946
S50	4.8782	0.0121	T50	4.6059

2.4 IC4 excited states

Table 9: Excited states of IC4

State	E [eV]	f	State	E [eV]
S1	2.4426	0.0159	T1	1.9270
S2	2.5266	0.0063	T2	1.9427
S3	2.7151	0.0009	T3	2.0157
S4	2.7345	0.0371	T4	2.1893
S5	2.7438	0.0105	T5	2.2523
S6	2.7875	0.0020	T6	2.2712
S7	2.9162	0.0408	T7	2.3622
S8	2.9452	0.0118	T8	2.5147
S9	3.0379	0.0224	T9	2.5244
S10	3.3261	0.0049	T10	2.5471
S11	3.3362	0.0204	T11	2.7888
S12	3.3926	0.0032	T12	2.8035
S13	3.4551	0.0008	T13	2.9177
S14	3.5807	0.0525	T14	3.1072
S15	3.5924	0.0013	T15	3.1937
S16	3.7774	0.0000	T16	3.2394
S17	3.8493	0.0003	T17	3.2517
S18	3.8581	0.0103	T18	3.3027
S19	3.8990	0.0300	T19	3.4835
S20	3.9966	0.0207	T20	3.5044
S21	4.0299	0.0667	T21	3.6205
S22	4.0450	0.0665	T22	3.6594
S23	4.0841	0.0028	T23	3.8130
S24	4.0976	0.0022	T24	3.9136
S25	4.1092	0.0822	T25	3.9643
S26	4.2002	0.0010	T26	3.9799
S27	4.3276	0.2041	T27	4.0164
S28	4.3438	0.2768	T28	4.0299
S29	4.4877	0.0647	T29	4.0322
S30	4.5047	0.0756	T30	4.0412
S31	4.6366	0.0400	T31	4.1474
S32	4.6436	0.0027	T32	4.1519
S33	4.7274	0.0377	T33	4.2222
S34	4.7285	0.1156	T34	4.2543
S35	4.8271	0.0342	T35	4.3332
S36	4.8430	0.0244	T36	4.3639
S37	4.9587	0.0027	T37	4.4473
S38	4.9617	0.0017	T38	4.4925
S39	5.0087	0.0011	T39	4.4976
S40	5.0321	0.0832	T40	4.5108
S41	5.0765	0.0933	T41	4.5647
S42	5.0930	0.0348	T42	4.6718
S43	5.1183	0.0063	T43	4.6767
S44	5.1372	0.0742	T44	4.7032
S45	5.1684	0.0508	T45	4.7778
S46	5.1890	0.0006	T46	4.7880
S47	5.2261	0.0318	T47	4.7982
S48	5.2946	0.0137	T48	4.8395
S49	5.3084	0.0369	T49	4.9221
S50	5.3095	0.0170	T50	4.9616

2.5 IC5 excited states

Table 10: Excited states of IC5

State	E [eV]	f	State	E [eV]
S1	2.2270	0.0000	T1	1.3240
S2	2.5348	0.0055	T2	1.5867
S3	2.5370	0.0056	T3	1.5889
S4	2.6616	0.0045	T4	1.9958
S5	2.6623	0.0044	T5	1.9986
S6	2.7106	0.0000	T6	2.1251
S7	2.7167	0.0000	T7	2.3356
S8	2.8628	0.0747	T8	2.4108
S9	2.9307	0.0000	T9	2.4817
S10	3.0252	0.0160	T10	2.4822
S11	3.0265	0.0161	T11	2.6098
S12	3.0868	0.0567	T12	2.6695
S13	3.1535	0.0110	T13	2.6964
S14	3.1539	0.0110	T14	2.8523
S15	3.3948	0.0000	T15	2.9434
S16	3.4302	0.0011	T16	2.9438
S17	3.4332	0.0011	T17	3.1119
S18	3.6364	0.0000	T18	3.1124
S19	3.9659	0.1508	T19	3.2232
S20	3.9663	0.1495	T20	3.2769
S21	4.0103	0.0287	T21	3.3621
S22	4.0781	0.0004	T22	3.3628
S23	4.0786	0.0003	T23	3.7551
S24	4.1202	0.0055	T24	3.7873
S25	4.1205	0.0056	T25	3.8270
S26	4.1492	0.1021	T26	3.8271
S27	4.1496	0.1034	T27	4.0049
S28	4.1824	0.0000	T28	4.0049
S29	4.1833	0.0002	T29	4.0315
S30	4.1860	0.0008	T30	4.0340
S31	4.1935	0.0033	T31	4.0417
S32	4.2018	0.2288	T32	4.0421
S33	4.2022	0.2296	T33	4.1589
S34	4.2853	0.0000	T34	4.1602
S35	4.3929	0.0000	T35	4.1606
S36	4.4126	0.0030	T36	4.1707
S37	4.4807	0.3507	T37	4.1715
S38	4.4823	0.0307	T38	4.1760
S39	4.8557	0.0061	T39	4.1828
S40	4.8564	0.0060	T40	4.1830
S41	4.9351	0.0000	T41	4.2980
S42	4.9376	0.0000	T42	4.3192
S43	4.9406	0.0000	T43	4.4361
S44	4.9435	0.0013	T44	4.4363
S45	4.9534	0.0000	T45	4.4471
S46	4.9673	0.0000	T46	4.4576
S47	5.0417	0.3464	T47	4.5002
S48	5.0556	0.0000	T48	4.5009
S49	5.0652	0.2071	T49	4.5781
S50	5.0655	0.2075	T50	4.5787

2.6 CASPT2 calculations for IC4 and IC5

Table 11: CASPT2 configuration information for the excited states of **4** selected for comparison with TDDFT results. Orbitals of active space are listed in the following order: symmetry 1: (σ_d, 3d, 3d, 4d, σ_d^*, π^*, 4d); symmetry 2: (σ_d, 3d, π^*, σ_d^*, 4d).

state	sym1	sym2	weight
4 S MLCT	22u00d0	22000	0.75
4 S MC	2220u00	2d000	0.48
	22200u0	2d000	0.37
4 T MLCT	2u200u0	22000	0.38
	2u20u00	22000	0.25
	2220000	2u0u0	0.13
4 T MC	22u0000	220u0	0.38
	2220u00	2u000	0.25
	2u20000	220u0	0.19

Table 12: Configuration information for the excited states of **5** selected for comparison with TDDFT results. Orbitals of active space are listed in the following order: symmetry 1: (σ_d, 3d, 4d, σ_d^*, π^*); symmetry 2: (3d, π^*, 4d); symmetry 3: (σ_d, σ_d^*); symmetry 4: (3d, 4d).

state	sym1	sym2	sym3	sym4	weight
5 S MLCT	22000	2u0	20	d0	0.60
	2u000	200	2d	20	0.29
5 S MC	2u000	200	2d	20	0.58
	22000	2u0	20	d0	0.29
5 T MLCT	22000	2u0	20	u0	0.88
5 T MC	2u000	200	2u	20	0.84