

RSC Advances

Theoretical study of the optical and charge transport properties of π -conjugated three-coordinate organoboron compounds as organic light-emitting materials

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Table S1 The Cartesian coordinates of **1–8** in S_0 at the PBE0/6-31G(d,p) level.

Table S2 The Cartesian coordinates of **1–8** in S_1 at the TD-PBE0/6-31G(d,p) level.

Table S3 The fluorescence (λ_{fl}) wavelengths (in nm), the oscillator strength f , main assignments (coefficient), and main electronic transitions of **5** at the TD-PBE0/6-31+G(d,p)//TD-PBE0/6-31(d,p) level and discussion.

Table S4 The calculated total energies of the compounds under investigation in different space groups.

Table S5 The calculated crystal cell parameters of the compounds under investigation with the lowest total energies.

Table S6 Center-center distance and the corresponding hole and electron coupling between the dimer in all of the nearest neighbor pathways for **1–6** in different space groups.

Table SI The Cartesian coordinates of **1–8** in S0 at the PBE0/6-31G(d,p) level.

1			
C	0.00000000	0.00000000	0.00000000
C	1.38317621	0.00000000	0.00000000
C	2.10604367	1.20821264	0.00000000
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C	-0.74988229	1.19503580	-0.02061636
H	-0.53069406	-0.94895029	0.01154022
H	1.91229200	-0.94851414	0.00519783
H	1.90346627	3.35177640	-0.00346130
H	-0.55665046	3.34127964	-0.04786133
C	5.87230464	0.29879130	0.00442424
C	6.60770198	-0.89582414	-0.01127617
C	6.61560627	1.49075737	0.02851879
C	7.99156989	-0.91642819	-0.00852824
H	6.07196612	-1.84247015	-0.02288251
C	7.99711824	1.49213839	0.03088698
H	6.10236420	2.44784051	0.04960617
C	8.73033160	0.28427850	0.00314251
H	8.49958727	-1.87351425	-0.01496309
H	8.51516192	2.44367923	0.05617615
N	10.10557444	0.28293755	-0.01589228
C	10.81970212	-0.96594055	0.08966205
H	11.89161516	-0.77263196	0.03276427
H	10.61695995	-1.49095026	1.03516244
H	10.56237303	-1.64247272	-0.73454291
C	10.82625218	1.52363460	0.13490293
H	11.89721497	1.32551281	0.07667007
H	10.57783929	2.22944714	-0.66718918
H	10.62265132	2.01743441	1.09677201
B	-2.31274664	1.18649586	-0.03376988
C	-3.07865349	-0.13590787	0.38022443
C	-3.94486489	-0.77682486	-0.54333681
C	-2.90419840	-0.73830561	1.64582227
C	-4.57706195	-1.96835762	-0.20167631
C	-3.56993321	-1.92860939	1.95758505
C	-4.40595821	-2.56485894	1.04920859
H	-5.22479659	-2.44796192	-0.93375933
H	-3.42650510	-2.36542955	2.94483444
C	-3.08260083	2.50070668	-0.46614071
C	-3.97601887	3.13608697	0.43533584
C	-2.88696127	3.09945876	-1.72996776
C	-4.61689428	4.31662753	0.07372262
C	-3.56161742	4.27935261	-2.06258259
C	-4.42741361	4.90786379	-1.17746849
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H	-4.87311309	-0.84789387	-2.48498986
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H	-6.16428557	-3.81063719	1.15046127
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H	-1.39467310	1.67527000	-2.42981863
H	-2.64825975	2.07762441	-3.60845661
H	-1.36757928	3.23451327	-3.25582251
C	-4.22454631	2.58351708	1.81452326
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H	-3.30812234	2.57514522	2.41543544
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H	-6.22717476	6.05465089	-1.49062319
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H	-1.36331048	1.65966290	-2.42994999
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H	-5.23013632	4.85632424	0.68594323
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H	-4.65198143	0.72495996	-1.79784207
H	-3.32751080	-0.25228980	-2.42367170
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H	-4.89459294	-4.00216516	2.72389537
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H	-3.28626175	2.66492119	2.37229390
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H	-6.17415583	6.00572795	-1.76430910
H	-4.92567546	6.95554147	-0.96285143
H	-4.74248261	6.51536841	-2.66762194
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S	4.49627571	2.59152468	-0.42313509
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H	4.78926751	4.79124756	0.32263629
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H	6.23962572	6.73677841	0.46359965
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H	10.63853422	5.99633138	1.39350375
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H	-3.41519379	4.67102489	-3.08262143
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H	-1.39425669	0.76471892	2.38362965
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H	-1.35366988	1.69237509	-2.42250883
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H	-1.46199598	3.18958550	-3.35354054
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H	4.29372790	-0.84723975	-0.09641128
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H	8.14641458	1.55830478	1.14770994
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N	9.66031441	5.84823463	1.52786039
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H	11.55802605	6.26231383	2.25682125
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C	9.31859697	7.24802140	1.59431882
H	10.21371944	7.82478755	1.83116598
H	8.94131895	7.61087202	0.63060527
H	8.55825702	7.46616253	2.36004760
B	-2.31047955	1.18800619	-0.02376032
C	-3.07738880	-0.14187998	0.36370313
C	-3.93848107	-0.76626505	-0.57632095
C	-2.90886306	-0.76804793	1.61829550
C	-4.57297554	-1.96327033	-0.26012155
C	-3.57615750	-1.96420946	1.90430637
C	-4.40887053	-2.58247575	0.98090852
H	-5.21535140	-2.42986024	-1.00529919
H	-3.43631812	-2.42084297	2.88304803
C	-3.08019981	2.50992098	-0.43472992
C	-3.97357825	3.12779304	0.47878155
C	-2.88351524	3.13426981	-1.68641116
C	-4.61096658	4.31759921	0.14169979
C	-3.55498503	4.32264688	-1.99437981
C	-4.41955313	4.93459306	-1.09651151
H	-5.27842148	4.77993893	0.86720096
H	-3.39306136	4.77756057	-2.97055860
C	-2.08604336	-0.16481719	2.72915149
H	-2.73915999	0.27213293	3.49460262
H	-1.47916937	-0.92884665	3.22581830
H	-1.41337354	0.61989125	2.38029039
C	-4.16076751	-0.18343896	-1.94753744
H	-4.85942078	-0.79701905	-2.52289539
H	-4.56405117	0.83199611	-1.89278525
H	-3.22730754	-0.12756320	-2.51860702
C	-5.11305498	-3.87177579	1.29651376
H	-6.20034932	-3.75929198	1.22101283
H	-4.82388255	-4.66423195	0.59721457
H	-4.88131150	-4.21667793	2.30771020
C	-2.02280611	2.53830153	-2.77255535
H	-1.37086958	1.74333408	-2.40861150
H	-2.64948751	2.11816338	-3.56873573
H	-1.39011081	3.30328034	-3.23459607
C	-4.22902350	2.54528791	1.84443767
H	-4.62950401	1.52914053	1.77959347
H	-3.30996668	2.49079802	2.43856078
H	-4.94304029	3.15814466	2.40137431
C	-5.13365632	6.21168788	-1.43847326
H	-6.21932569	6.06427178	-1.46466342
H	-4.93440318	6.99098836	-0.69478152
H	-4.82519146	6.59271615	-2.41561838
C	3.55366576	1.19805496	0.00055994
C	4.45601820	0.19665983	-0.33280231
C	5.75628272	0.71087994	-0.17059550
H	4.19373850	-0.78411950	-0.70424507
C	5.64273320	2.02457884	0.26523171
H	6.68497651	0.20431276	-0.39282606
N	4.30354270	2.30085304	0.34048694
H	3.92960192	3.11863393	0.79222667

6

C	0.00000000	0.00000000	0.00000000
C	1.38714047	0.00000000	0.00000000
C	2.10407027	1.20706983	0.00000000

C	1.37730029	2.40709169	-0.01797159
C	-0.00944010	2.39779926	-0.04371656
C	-0.74205884	1.19593058	-0.02862488
H	-0.53276620	-0.94734111	0.02979543
H	1.92981388	-0.94005148	0.04085624
H	1.91718313	3.34994607	-0.03890438
H	-0.54914572	3.34096183	-0.07880680
C	7.92307326	1.24798768	0.55469696
C	8.65739277	0.06210493	0.68656390
C	8.63294502	2.44820884	0.68178363
C	10.02254642	0.06807335	0.92575571
H	8.14014558	-0.89205533	0.63792145
C	9.99833698	2.47327422	0.91666044
H	8.10076472	3.38976170	0.57480670
C	10.73731872	1.27845712	1.03345473
H	10.53215584	-0.88106393	1.04342884
H	10.49343486	3.43366655	0.99997556
N	12.10183211	1.29315711	1.23780688
C	12.78552352	0.05884747	1.53811760
H	13.85372749	0.25653994	1.63882232
H	12.43439407	-0.41111346	2.46997711
H	12.66265835	-0.66729681	0.72613457
C	12.75645201	2.54043015	1.55016490
H	13.82642060	2.36334102	1.66874685
H	12.63319299	3.26593732	0.73751647
H	12.38047703	3.00141141	2.47660509
B	-2.30941391	1.19194660	-0.03211208
C	-3.07014737	-0.10787965	0.45023950
C	-3.95812047	-0.78314851	-0.42731014
C	-2.86545286	-0.66000887	1.73433309
C	-4.58112938	-1.96024884	-0.02472778
C	-3.52313655	-1.83697457	2.10742576
C	-4.38090719	-2.50680841	1.24478601
H	-5.24344698	-2.46928130	-0.72312521
H	-3.35556376	-2.23672351	3.10648376
C	-3.07399870	2.49085058	-0.51102366
C	-3.95872546	3.16325670	0.37179195
C	-2.87588801	3.04545310	-1.79476245
C	-4.58268039	4.34162583	-0.02533122
C	-3.53459228	4.22343299	-2.16270856
C	-4.38665856	4.89242704	-1.29372710
H	-5.24362140	4.84836005	0.67602448
H	-3.37189467	4.62409275	-3.16217284
C	-2.01371170	0.00620203	2.78568687
H	-2.64716292	0.46819867	3.55286234
H	-1.37731468	-0.72488832	3.29483123
H	-1.36592293	0.78332639	2.37820612
C	-4.22100294	-0.28009006	-1.82307899
H	-4.93991377	-0.92285359	-2.33828934
H	-4.61864259	0.73902945	-1.81559829
H	-3.30605289	-0.26377280	-2.42591714
C	-5.08019655	-3.77136363	1.65644043
H	-6.16573334	-3.62713143	1.70173443
H	-4.89413359	-4.57983563	0.94126876
H	-4.74736597	-4.10960187	2.64121246
C	-2.03026441	2.37773419	-2.84997523
H	-1.37933974	1.60295778	-2.44266023
H	-2.66789574	1.91105955	-3.61079226
H	-1.39861083	3.10777313	-3.36645749
C	-4.22075530	2.65316592	1.76517582
H	-4.63832886	1.64201287	1.75139857
H	-3.30211642	2.61287486	2.36099341
H	-4.92340533	3.30512645	2.29115780
C	-5.07248622	6.16865390	-1.69147482
H	-6.15504031	6.10320766	-1.53822493
H	-4.71459537	7.01379524	-1.09232107
H	-4.89502736	6.40756251	-2.74339235

C	5.64317212	2.08325320	1.06535073
C	6.46359493	1.24601108	0.34782378
C	4.23121043	2.07609296	0.92175893
H	6.08529470	2.73820152	1.81092448
C	5.83398363	0.37894112	-0.61359900
C	3.57777935	1.22581446	0.06268548
H	3.64264533	2.72803607	1.56151782
C	4.39027618	0.36369048	-0.75440584
C	6.44868991	-0.45912309	-1.52801625
C	3.98169785	-0.48750403	-1.76677667
H	7.50656205	-0.61850024	-1.67652221
H	2.97660347	-0.67681434	-2.11412653
S	5.30939130	-1.24036971	-2.52211816

7

C	0.00000000	0.00000000	0.00000000
C	1.38695198	0.00000000	0.00000000
C	2.09912828	1.20939644	0.00000000
C	1.36822109	2.40811887	-0.03132959
C	-0.01741437	2.39667412	-0.05855096
C	-0.74608943	1.19277875	-0.03367319
H	-0.52971451	-0.94898002	0.02500980
H	1.92995710	-0.93803904	0.00861953
H	1.89979552	3.35497348	-0.07041687
H	-0.55818267	3.33856509	-0.10603094
C	7.96486424	1.54131752	0.33903697
C	8.82396214	0.43249070	0.35570122
C	8.56204499	2.80489609	0.45959131
C	10.19313915	0.57360869	0.50003365
H	8.40859778	-0.56404061	0.26136219
C	9.92932753	2.96385888	0.59819995
H	7.94117982	3.69551469	0.41439054
C	10.78968305	1.84600807	0.61994263
H	10.80431139	-0.32088353	0.52373153
H	10.33113462	3.96726454	0.67561268
N	12.15171419	1.99251290	0.74185462
C	12.98812253	0.82455918	0.87402558
H	14.03222077	1.13518986	0.92920416
H	12.75790825	0.23901085	1.77666289
H	12.88642056	0.16176016	0.00607055
C	12.70991708	3.29637001	1.00481082
H	13.79586924	3.21627498	1.06700884
H	12.47739395	4.00184053	0.19733104
H	12.34554878	3.72919357	1.94835161
B	-2.31406641	1.18224740	-0.04988427
C	-3.07159213	-0.11637695	0.43925112
C	-3.94851439	-0.80511552	-0.43871608
C	-2.87227909	-0.65586534	1.72961871
C	-4.56360024	-1.98485655	-0.03099207
C	-3.52200982	-1.83533650	2.10764479
C	-4.36524639	-2.52117909	1.24286790
H	-5.21931426	-2.50362839	-0.72842299
H	-3.36054233	-2.22394736	3.11208003
C	-3.07720837	2.47252818	-0.55256125
C	-3.97135760	3.15519338	0.31247291
C	-2.86219350	3.01326852	-1.83968572
C	-4.58818343	4.33089690	-0.10407647
C	-3.51323616	4.18918212	-2.22689278
C	-4.37604868	4.86760561	-1.37568374
H	-5.25480777	4.84708738	0.58487206
H	-3.33616929	4.58124383	-3.22737279
C	-2.03797456	0.03033721	2.78200106
H	-2.68379294	0.50383088	3.53170882
H	-1.40694464	-0.68983778	3.31283340
H	-1.38693923	0.80290218	2.37066883
C	-4.21046663	-0.31304975	-1.83858678
H	-4.92239024	-0.96503070	-2.35191322

H	-4.61650792	0.70278601	-1.83895297
H	-3.29366820	-0.29342937	-2.43853371
C	-5.03504049	-3.80288898	1.65037149
H	-6.10519557	-3.78439909	1.41910554
H	-4.60626426	-4.65956618	1.11732718
H	-4.92347339	-3.98955709	2.72171832
C	-2.00493306	2.33329575	-2.87735886
H	-1.35917338	1.56184783	-2.45569074
H	-2.63455012	1.85957109	-3.64045122
H	-1.36641401	3.05687210	-3.39446977
C	-4.24812634	2.66113516	1.70875520
H	-4.64795321	1.64285145	1.70275633
H	-3.33887851	2.64531790	2.32019208
H	-4.97031008	3.30841029	2.21364929
C	-5.07189501	6.12850810	-1.80420886
H	-6.14993461	5.96624764	-1.91905507
H	-4.94492435	6.92506681	-1.06352044
H	-4.68704646	6.49205616	-2.76065916
C	5.64979053	2.31077857	0.84540710
C	6.50557911	1.41344001	0.23843141
C	4.23978322	2.23407565	0.75532703
H	6.07342961	3.10182304	1.45651819
C	5.85648035	0.36448932	-0.49735828
C	3.57024776	1.24766453	0.06267890
H	3.65809008	2.97408199	1.29749393
C	4.40926763	0.27999117	-0.58027752
S	5.31454575	-1.51552571	-1.85748475
N	3.98658192	-0.74465324	-1.32465321
N	6.47473806	-0.59858674	-1.18450870

8

C	0.00000000	0.00000000	0.00000000
C	1.38675467	0.00000000	0.00000000
C	2.09876186	1.20879533	0.00000000
C	1.36936788	2.40762015	-0.02631692
C	-0.01690286	2.39710756	-0.05439555
C	-0.74567638	1.19357584	-0.03199188
H	-0.53024360	-0.94873900	0.02401021
H	1.93183294	-0.93682541	0.00501547
H	1.90231446	3.35402315	-0.05803597
H	-0.55729090	3.33944412	-0.09774441
C	7.92229290	1.51279399	0.35323828
C	8.74733889	0.39680834	0.53847364
C	8.54801859	2.76465966	0.30795386
C	10.12227574	0.51638797	0.66312660
H	8.30331445	-0.59106669	0.62498004
C	9.92082331	2.90286373	0.42698758
H	7.94342732	3.65455064	0.15389027
C	10.75208097	1.77610982	0.59709894
H	10.70741765	-0.38082526	0.82659719
H	10.34897312	3.89707576	0.37646118
N	12.12036741	1.90154272	0.69044412
C	12.92098027	0.74548493	1.01246919
H	13.97481237	1.02725727	1.00983052
H	12.68218155	0.32272704	2.00030030
H	12.79083641	-0.04616130	0.26503678
C	12.70874376	3.21437553	0.79728586
H	13.79360323	3.11721394	0.85582561
H	12.48110246	3.82537505	-0.08459633
H	12.36631161	3.76288938	1.68785150
B	-2.31287127	1.18361493	-0.04583006
C	-3.07094228	-0.11628459	0.44081490
C	-3.94690734	-0.80371456	-0.43890978
C	-2.87321529	-0.65768624	1.73063195
C	-4.56369290	-1.98328259	-0.03319516
C	-3.52451421	-1.83700095	2.10669888
C	-4.36759247	-2.52101674	1.24038803

H	-5.21892998	-2.50093179	-0.73193478
H	-3.36388023	-2.22705695	3.11073101
C	-3.07834249	2.47519877	-0.54332099
C	-3.97067304	3.15465792	0.32602195
C	-2.86777812	3.01999799	-1.82957823
C	-4.59082259	4.33032443	-0.08573364
C	-3.52196560	4.19584575	-2.21182388
C	-4.38364380	4.87056285	-1.35660528
H	-5.25594862	4.84393092	0.60661746
H	-3.34753535	4.59099461	-3.21155346
C	-2.03772229	0.02553912	2.78405143
H	-2.68260427	0.49991106	3.53402120
H	-1.40866862	-0.69681460	3.31427903
H	-1.38452848	0.79641575	2.37308995
C	-4.20562508	-0.31029006	-1.83886322
H	-4.91726506	-0.96102360	-2.35420807
H	-4.61024382	0.70611751	-1.83925609
H	-3.28736901	-0.29125509	-2.43656138
C	-5.03919377	-3.80248012	1.64577630
H	-6.10905457	-3.78277041	1.41316111
H	-4.61056991	-4.65918961	1.11262372
H	-4.92935286	-3.99030076	2.71713881
C	-2.01176882	2.34483976	-2.87143821
H	-1.35407453	1.58268311	-2.45144292
H	-2.64238040	1.86087358	-3.62732611
H	-1.38577174	3.07334896	-3.39678820
C	-4.24178727	2.65768499	1.72239393
H	-4.64207348	1.63956402	1.71614960
H	-3.32985916	2.64028901	2.32970498
H	-4.96152173	3.30430696	2.23164453
C	-5.08310176	6.13128369	-1.77978716
H	-6.16107716	5.96711590	-1.89271108
H	-4.95615765	6.92593573	-1.03703129
H	-4.70131174	6.49862075	-2.73605188
C	5.61423732	2.29598639	0.90882085
C	6.45595501	1.40051923	0.24585550
C	4.22453861	2.22194120	0.81940753
H	6.06361717	3.05373164	1.54395952
C	5.80708779	0.41821251	-0.52023362
C	3.57312508	1.24680453	0.06469932
H	3.62618677	2.92656362	1.38908748
C	4.39920985	0.32761971	-0.62115831
N	3.93719751	-0.66655329	-1.46202727
C	4.92267524	-1.30858460	-1.98868366
H	4.79671750	-2.13407970	-2.68133967
S	6.52715634	-0.79667258	-1.54155065

Table S2 The Cartesian coordinates of **1–8** in S1 at the TD-PBE0/6-31G(d,p) level.

1			
C	0.44794500	0.90593700	-0.38980100
C	-0.92648600	0.82084100	-0.36446600
C	-1.57373500	-0.33720600	0.14021300
C	-0.75099300	-1.39010700	0.60691700
C	0.62461200	-1.29404000	0.57561200
C	1.28877900	-0.14131900	0.07609000
H	0.91845500	1.80213700	-0.78734700
H	-1.51842400	1.65100200	-0.74118600
H	-1.22414000	-2.28858700	1.00002200
H	1.22844300	-2.11774200	0.94825800
C	-5.36884600	0.23368500	-0.12436000
C	-6.23951300	1.26931800	-0.54818900
C	-5.99031700	-0.95191000	0.35001200
C	-7.60844800	1.14749600	-0.50535400
H	-5.80443300	2.19298300	-0.91999600
C	-7.35757900	-1.08846800	0.39992800
H	-5.37852800	-1.78284800	0.68496800

C	-8.21607000	-0.04211800	-0.02616600
H	-8.21945200	1.97543700	-0.84454500
H	-7.77451300	-2.01652600	0.77263600
N	-9.57443600	-0.17461700	0.02197900
C	-10.42945800	0.90562000	-0.41842100
H	-11.47130400	0.61248700	-0.29496600
H	-10.26025400	1.81678200	0.16887400
H	-10.26509300	1.14318800	-1.47708200
C	-10.17152200	-1.39907300	0.50752000
H	-11.25649000	-1.31193400	0.46415500
H	-9.87391400	-2.26098500	-0.10288800
H	-9.88678100	-1.60007800	1.54803100
B	2.84767500	-0.02545500	0.03114300
C	3.50858300	1.41006200	-0.02062200
C	4.48128600	1.73142200	-1.00739900
C	3.17249500	2.42868100	0.90931600
C	5.04261900	3.00523500	-1.06242800
C	3.76817500	3.68889400	0.83136500
C	4.69997100	4.00638900	-0.15285400
H	5.77300700	3.22485100	-1.84018400
H	3.50373200	4.44246300	1.57245600
C	3.72208400	-1.34229100	0.03606600
C	4.79194000	-1.50617200	0.95861700
C	3.49288900	-2.40120200	-0.88181100
C	5.55033800	-2.67473200	0.96505900
C	4.28483600	-3.55034400	-0.85464600
C	5.31524100	-3.71624700	0.06675800
H	6.35295900	-2.77619200	1.69462600
H	4.09710600	-4.33608200	-1.58560700
C	2.20110800	2.19178200	2.03791000
H	2.39320400	2.88272100	2.86504900
H	1.16227500	2.33903100	1.71964700
H	2.26286500	1.16933600	2.42149500
C	4.92014700	0.72513100	-2.03942800
H	5.55755100	1.19583200	-2.79418600
H	5.47898300	-0.10121700	-1.58940600
H	4.06383500	0.27647300	-2.55373000
C	5.30649400	5.37799600	-0.24390900
H	6.37112400	5.33028700	-0.49524900
H	4.81980400	5.97885600	-1.02261500
H	5.20536600	5.92310300	0.69924600
C	2.42608200	-2.31870100	-1.94335300
H	2.31281600	-1.30118100	-2.32897100
H	2.66108400	-2.98150700	-2.78226600
H	1.44315400	-2.61127900	-1.55550800
C	5.12860500	-0.44366300	1.97254800
H	5.52015200	0.46143400	1.49805700
H	4.24559300	-0.13742100	2.54330900
H	5.87817700	-0.80762900	2.68189300
C	6.13609000	-4.97418400	0.10552400
H	7.18960000	-4.75960800	0.31244500
H	5.78671800	-5.65478900	0.89233400
H	6.08079100	-5.51696100	-0.84273900
C	-2.99829400	-0.48236000	0.19678800
C	-3.94990100	0.42903000	-0.19462300
H	-3.33975900	-1.43398000	0.60338600
H	-3.62597900	1.38743400	-0.59248000

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C	1.44838500	1.13404700	-0.39300600
C	0.06908100	1.13571200	-0.40416900
C	-0.67031300	-0.00014800	-0.00021800
C	0.06911700	-1.13595300	0.40381400
C	1.44842100	-1.13418700	0.39280300
C	2.21166900	-0.00003900	-0.00004900
H	1.98070300	2.02993400	-0.70428000
H	-0.45454300	2.04391700	-0.69316400

H	-0.45448000	-2.04419100	0.69276300
H	1.98077500	-2.03003400	0.70413200
C	-6.44252600	-0.00012500	-0.00019000
C	-7.18737000	1.14259500	-0.38046400
C	-7.18741600	-1.14277800	0.38019200
C	-8.56174100	1.15231200	-0.38424400
H	-6.66016600	2.05232600	-0.64563700
C	-8.56178700	-1.15233600	0.38426900
H	-6.66025100	-2.05257900	0.64520800
C	-9.29774100	0.00004600	0.00013900
H	-9.07855500	2.06090100	-0.66813200
H	-9.07864300	-2.06089900	0.66816300
N	-10.65869400	0.00016500	0.00035700
C	-11.39297000	1.17695500	-0.42011300
H	-12.46039200	0.96677000	-0.38120100
H	-11.18656700	2.03046800	0.23619300
H	-11.13573000	1.45698700	-1.44768500
C	-11.39307200	-1.17656500	0.42081800
H	-12.46044400	-0.96593400	0.38293800
H	-11.18756100	-2.02984100	-0.23608800
H	-11.13508000	-1.45720000	1.44802800
B	3.76313900	0.00002200	0.00003100
C	4.54500100	1.38168300	-0.01272300
C	5.54881500	1.64811400	-0.98371900
C	4.29424000	2.39692800	0.94549100
C	6.22778200	2.86424700	-0.99315800
C	5.00528300	3.59980600	0.91347400
C	5.97295600	3.86149300	-0.05064200
H	6.98120400	3.04002500	-1.76040300
H	4.80066200	4.35138600	1.67543700
C	4.54513300	-1.38155900	0.01282100
C	5.54889700	-1.64796400	0.98388200
C	4.29445700	-2.39682400	-0.94540200
C	6.22792100	-2.86406300	0.99334900
C	5.00555800	-3.59966600	-0.91335400
C	5.97319600	-3.86131300	0.05080900
H	6.98129600	-3.03981200	1.76064500
H	4.80100800	-4.35125500	-1.67532800
C	3.28599300	2.22168300	2.05249600
H	3.53567100	2.85721100	2.90842600
H	2.27383600	2.48762900	1.72514400
H	3.23120700	1.18402700	2.39278700
C	5.89505100	0.63976200	-2.04796400
H	6.59441300	1.06419000	-2.77505600
H	6.34917000	-0.25987800	-1.62161300
H	5.00298600	0.30932700	-2.59060300
C	6.71475300	5.16826300	-0.08519000
H	7.79627500	5.01464700	-0.16987400
H	6.41118700	5.77928000	-0.94433400
H	6.52890900	5.75612300	0.81852400
C	3.28624800	-2.22164700	-2.05245300
H	3.23128300	-1.18396400	-2.39263100
H	3.53611000	-2.85703300	-2.90843700
H	2.27412100	-2.48783100	-1.72519900
C	5.89498800	-0.63963900	2.04820000
H	6.34915400	0.26001200	1.62192600
H	5.00285500	-0.30922900	2.59074000
H	6.59426600	-1.06408000	2.77536700
C	6.71501800	-5.16806700	0.08541200
H	7.79650100	-5.01443400	0.17054900
H	6.41113000	-5.77924900	0.94432500
H	6.52953900	-5.75577200	-0.81847900
C	-2.12768100	-0.00017800	-0.00025800
C	-2.87300700	0.85664400	-0.84616000
C	-2.87300900	-0.85705300	0.84558300
C	-4.25173300	0.86684500	-0.83594900
H	-2.34554100	1.49789900	-1.54392500

C	-4.25173900	-0.86724100	0.83537400
H	-2.34554700	-1.49835500	1.54330900
C	-4.98709800	-0.00017700	-0.00026600
H	-4.77407800	1.51852800	-1.53105600
H	-4.77409000	-1.51895900	1.53044500

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C	-1.56579100	-1.46388800	-0.57132100
C	-0.21610400	-1.72824700	-0.66153300
C	0.74311400	-0.75251400	-0.29251600
C	0.25765200	0.49787800	0.16013200
C	-1.09488200	0.75039600	0.23866500
C	-2.07176500	-0.21701400	-0.11771900
H	-2.27611700	-2.23216400	-0.86723900
H	0.11235100	-2.69699600	-1.02727300
H	0.96175900	1.27161500	0.46052800
H	-1.43412200	1.71871000	0.59849600
C	6.03726600	-0.51521900	-0.14540300
C	7.11431300	-1.39826100	-0.41458200
C	6.38482100	0.78675100	0.29497600
C	8.42512300	-1.01836100	-0.25629000
H	6.90595700	-2.40651300	-0.75598100
C	7.69325400	1.17849700	0.45782900
H	5.59797200	1.50255800	0.51400300
C	8.76167700	0.28707400	0.18836800
H	9.20530000	-1.73679600	-0.47736900
H	7.89575900	2.18683700	0.79815100
N	10.06226000	0.66742200	0.34993500
C	11.13516500	-0.26130600	0.06941500
H	12.09076200	0.22635100	0.25836300
H	11.07511500	-1.15106100	0.70871300
H	11.12145400	-0.58804800	-0.97795500
C	10.37912900	2.00296400	0.80664600
H	11.46086200	2.11262700	0.87349900
H	10.00172600	2.76510200	0.11345000
H	9.95462900	2.19975500	1.79908400
B	-3.59878000	0.06830100	-0.01322000
C	-4.60628300	-1.15144100	0.05776700
C	-5.70297200	-1.24927800	-0.83950200
C	-4.46233900	-2.18295300	1.02044000
C	-6.57405400	-2.33526600	-0.77931500
C	-5.36656400	-3.24639400	1.06199900
C	-6.42579100	-3.35104100	0.16523700
H	-7.39740200	-2.38875800	-1.49052600
H	-5.24282300	-4.01241500	1.82675200
C	-4.10686600	1.56761800	0.02102300
C	-4.97455500	2.02510000	1.04998400
C	-3.72677000	2.50721300	-0.97015000
C	-5.39905400	3.35103700	1.08213700
C	-4.18732000	3.82529700	-0.91379300
C	-5.01888900	4.27415100	0.10654100
H	-6.04878300	3.67560900	1.89401600
H	-3.89193800	4.51971100	-1.69950100
C	-3.36562800	-2.16722300	2.05547000
H	-3.66901400	-2.72248900	2.94884900
H	-2.44519100	-2.62719700	1.67709100
H	-3.09917300	-1.15025100	2.35522800
C	-5.95069200	-0.20407000	-1.89624000
H	-6.76803000	-0.50619100	-2.55798400
H	-6.20842200	0.76386300	-1.45582000
H	-5.06269900	-0.03817000	-2.51536200
C	-7.36733500	-4.52175000	0.19951300
H	-8.39564300	-4.21618000	-0.01884300
H	-7.09107000	-5.27714400	-0.54688700
H	-7.35989900	-5.01226000	1.17730600
C	-2.84760500	2.13374600	-2.13741900
H	-2.99874800	1.09703500	-2.44976500

H	-3.04653200	2.78501800	-2.99457200
H	-1.78357000	2.22888100	-1.89081500
C	-5.43947700	1.10973500	2.15295200
H	-6.05084100	0.28897800	1.76648500
H	-4.59529200	0.64992900	2.67826100
H	-6.03148600	1.65987100	2.89044600
C	-5.51010000	5.69360200	0.15346500
H	-6.59605700	5.74619800	0.01072900
H	-5.29297800	6.16029700	1.12088400
H	-5.04354600	6.30340800	-0.62530600
C	2.14977100	-1.03702400	-0.37598600
C	2.78563600	-2.22915400	-0.75776200
S	3.34531600	0.17013900	0.02555300
C	4.17532900	-2.15906200	-0.71885500
H	2.23823400	-3.11741800	-1.04494200
C	4.67628300	-0.92203800	-0.30867500
H	4.81434600	-2.99530800	-0.97948500

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C	-1.45157200	-1.70758300	-0.65158100
C	-0.15674700	-2.16476700	-0.79192000
C	0.93623300	-1.32691800	-0.48151000
C	0.66939700	-0.01763300	-0.03000900
C	-0.63218400	0.42461400	0.10255600
C	-1.75042700	-0.39570300	-0.19944300
H	-2.27860400	-2.36861400	-0.89894000
H	0.02140200	-3.17698500	-1.14664600
H	1.49795900	0.63982200	0.21660000
H	-0.81651500	1.43516900	0.45891000
C	5.68278900	-0.91572100	-0.22599200
C	6.95459600	-1.50965900	-0.41133800
C	5.64904000	0.41506700	0.25676000
C	8.11343300	-0.82717800	-0.13359400
H	7.02088800	-2.52772000	-0.78175900
C	6.80413100	1.10499600	0.53765500
H	4.68775200	0.89340200	0.40701200
C	8.07757300	0.50729000	0.35312500
H	9.06285400	-1.32379900	-0.29215700
H	6.72730700	2.12053000	0.90637500
N	9.22520000	1.18732700	0.63224100
C	10.51386900	0.55632500	0.44311700
H	11.30017100	1.25407700	0.72816100
H	10.61594100	-0.34245900	1.06358200
H	10.67384500	0.27356900	-0.60469500
C	9.16606200	2.54773500	1.12383600
H	10.17882700	2.91792200	1.27761900
H	8.66608800	3.21143400	0.40798400
H	8.63253300	2.60653000	2.08047800
B	-3.22405200	0.11018300	-0.03818500
C	-4.37793700	-0.95272000	0.15865100
C	-5.54870900	-0.92275500	-0.64735700
C	-4.30319200	-1.96958600	1.14746200
C	-6.55143400	-1.87613800	-0.48129400
C	-5.33464900	-2.89860600	1.29349600
C	-6.46667000	-2.88040100	0.48319200
H	-7.42867000	-1.83372000	-1.12594900
H	-5.25597300	-3.65361000	2.07518200
C	-3.51029900	1.66437600	-0.06794800
C	-4.28065700	2.28750900	0.95218500
C	-3.02514300	2.50126900	-1.10860100
C	-4.50991000	3.66194500	0.93156700
C	-3.28736900	3.87213700	-1.10205000
C	-4.01964200	4.48048300	-0.08590700
H	-5.09098900	4.10974500	1.73699500
H	-2.91827900	4.48191400	-1.92622500
C	-3.14383200	-2.06668700	2.10633300
H	-3.44315000	-2.58067200	3.02549100

H	-2.30248600	-2.62224800	1.67558800
H	-2.75460600	-1.07986100	2.37350600
C	-5.73844800	0.11871900	-1.71954900
H	-6.62167000	-0.10429900	-2.32604400
H	-5.86007700	1.12036800	-1.29551400
H	-4.87252600	0.16929900	-2.38813100
C	-7.55003400	-3.91162700	0.62836600
H	-8.53976500	-3.48300700	0.44074200
H	-7.41606500	-4.73556300	-0.08420800
H	-7.55485400	-4.34811100	1.63171700
C	-2.25385100	1.94958400	-2.28028500
H	-2.62133500	0.96340000	-2.57951000
H	-2.32557000	2.62091300	-3.14203400
H	-1.19038700	1.82230200	-2.04631200
C	-4.85414600	1.49821600	2.10034500
H	-5.64287400	0.81479600	1.77037800
H	-4.09125900	0.87912500	2.58390400
H	-5.27754600	2.16582700	2.85715500
C	-4.26029400	5.96371900	-0.07446600
H	-5.24589300	6.20697300	0.33526900
H	-3.51769500	6.48511100	0.54316500
H	-4.19875600	6.38680500	-1.08172900
C	2.28382100	-1.81036100	-0.62351500
C	2.81805000	-3.02924300	-1.04078900
C	4.21004500	-2.90555600	-0.96779000
H	2.25375900	-3.89360000	-1.35538400
C	4.48462800	-1.62449200	-0.50973400
H	4.94162800	-3.66126200	-1.21709400
O	3.29866400	-0.96869900	-0.30525900

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C	-0.02755400	0.04138200	-0.01623100
C	-0.03672900	0.04694900	1.36350400
C	1.17479900	0.04476600	2.08414300
C	2.38588800	0.03214000	1.36273400
C	2.37602000	0.02994100	-0.01682500
C	1.17412300	0.03761100	-0.78778400
H	-0.97780300	0.01979700	-0.54472900
H	-0.98421800	0.03811400	1.89884000
H	3.33372100	0.03209200	1.89749300
H	3.32600900	0.04054700	-0.54608900
C	1.19564000	2.15008800	6.52263000
C	1.20226400	1.87063700	7.91439800
C	1.20188500	3.51746700	6.14585500
C	1.21562100	2.86686000	8.85412000
H	1.19679300	0.83939300	8.24903900
C	1.21560200	4.52464700	7.07556000
H	1.19673800	3.79572800	5.09740200
C	1.22387400	4.23599400	8.46816700
H	1.22035700	2.59643300	9.90239100
H	1.22039500	5.55106300	6.73176000
N	1.23926000	5.22726600	9.39008300
C	1.24691200	4.91250200	10.80678900
H	1.25915900	5.83884900	11.37841200
H	0.35351000	4.34705600	11.09402200
H	2.13445400	4.33151500	11.08091200
C	1.24924000	6.61800000	8.97420600
H	1.26357000	7.25449700	9.85718300
H	2.13675000	6.84764900	8.37447400
H	0.35594000	6.86551400	8.39035200
B	1.17543400	0.03869300	-2.32802500
C	-0.15858100	0.40086900	-3.12069500
C	-0.68717500	-0.46812600	-4.11241400
C	-0.86401700	1.61115000	-2.89766100
C	-1.84960700	-0.14221600	-4.80887200
C	-2.02448300	1.91002300	-3.61855300
C	-2.54267100	1.04573900	-4.57653100

H	-2.22742800	-0.83896800	-5.55679700
H	-2.53027700	2.85752700	-3.43230500
C	2.51221600	-0.32299300	-3.11627600
C	3.05164800	0.55283500	-4.09634400
C	3.21239200	-1.53605400	-2.89526900
C	4.21828900	0.22954000	-4.78621400
C	4.37806100	-1.83221700	-3.60974900
C	4.90366500	-0.96466500	-4.56007900
H	4.60685200	0.93335900	-5.52207700
H	4.88237200	-2.78018700	-3.42277400
C	-0.38559500	2.64141700	-1.90669500
H	-0.75705400	3.63722500	-2.17125700
H	-0.72739200	2.41587500	-0.88900700
H	0.70659300	2.67230000	-1.85749000
C	-0.02225700	-1.78191100	-4.42889100
H	-0.61847000	-2.36174700	-5.14071100
H	0.97671300	-1.64004900	-4.85243200
H	0.10869200	-2.38648000	-3.52484900
C	-3.80671600	1.36764400	-5.32469200
H	-3.72574500	1.10140300	-6.38404100
H	-4.66565600	0.81646200	-4.92110000
H	-4.04593300	2.43380600	-5.26352600
C	2.72746900	-2.56951200	-1.91097500
H	1.63539500	-2.59252200	-1.85885500
H	3.08980500	-3.56642600	-2.18322500
H	3.07317700	-2.35588900	-0.89221400
C	2.39531800	1.87362000	-4.40211200
H	1.39501600	1.74167200	-4.82579500
H	2.26896600	2.47212700	-3.49312800
H	2.99462800	2.45512700	-5.11006500
C	6.14661000	-1.30511900	-5.33509200
H	5.91929200	-1.52142500	-6.38629900
H	6.86475500	-0.47734300	-5.32842600
H	6.64635500	-2.18529300	-4.91948900
C	1.17738500	0.09740800	3.54815000
C	1.18136400	-0.91685100	4.53618200
C	1.18603500	-0.31064800	5.77662600
H	1.18081500	-1.97345300	4.31608300
C	1.18582400	1.09610700	5.57648500
H	1.19029600	-0.80311600	6.73844200
N	1.17937100	1.27809600	4.20975400
H	1.17791400	2.15436400	3.71230600

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C	1.77116200	-1.01876300	0.17427600
C	0.39341300	-0.97317100	0.25142600
C	-0.31151200	0.23673300	0.04401600
C	0.45696600	1.38672400	-0.25776200
C	1.83470100	1.33275300	-0.30255800
C	2.55743500	0.13029900	-0.09351200
H	2.27802500	-1.97013400	0.32008200
H	-0.16352900	-1.89265300	0.40933700
H	-0.04799400	2.33768900	-0.40791100
H	2.39398000	2.24168500	-0.51268200
C	-6.11181000	0.34730600	-0.22870800
C	-6.87767900	-0.83171300	-0.08671200
C	-6.81488400	1.50617700	-0.63000900
C	-8.23781200	-0.85546700	-0.30885700
H	-6.37177400	-1.76105000	0.15441800
C	-8.17507200	1.50179900	-0.84881800
H	-6.27523300	2.44300100	-0.72994200
C	-8.93511100	0.31727600	-0.68869800
H	-8.76532600	-1.79721800	-0.21360200
H	-8.66106800	2.42760200	-1.13308900
N	-10.28491800	0.30478300	-0.90118000
C	-11.03637700	-0.91892800	-0.73540100
H	-12.09336500	-0.71756800	-0.90708300

H	-10.71772800	-1.69293500	-1.44606200
H	-10.92927800	-1.32029700	0.27978600
C	-10.96397000	1.50476000	-1.33611900
H	-12.02506100	1.29154500	-1.46205600
H	-10.86601500	2.31276200	-0.60004600
H	-10.57366800	1.86621000	-2.29616400
B	4.10750500	0.07542200	-0.16355100
C	4.82374100	-1.32448000	-0.36798600
C	5.81945100	-1.78116500	0.53569600
C	4.50219700	-2.16659600	-1.46015600
C	6.42815000	-3.02033400	0.35207500
C	5.14787900	-3.39587000	-1.62172600
C	6.10881200	-3.84876300	-0.72483600
H	7.17796000	-3.34912200	1.07062600
H	4.89385300	-4.01414400	-2.48194800
C	4.93726900	1.42052600	-0.02841600
C	5.88244500	1.80234200	-1.01673100
C	4.77357100	2.28483000	1.08169500
C	6.59290200	2.99438100	-0.89412100
C	5.51848600	3.46331000	1.17950100
C	6.42783800	3.84525800	0.19915700
H	7.30187900	3.26672800	-1.67488300
H	5.38562500	4.09774000	2.05498200
C	3.48666200	-1.78003600	-2.50679900
H	3.73392100	-2.23602700	-3.47084600
H	2.47885000	-2.11383300	-2.23332700
H	3.42522200	-0.69783800	-2.64355100
C	6.22707300	-0.96420600	1.73426700
H	6.97668600	-1.49395600	2.32943900
H	6.64341400	0.00427600	1.44241200
H	5.37278300	-0.75523600	2.38765900
C	6.79000400	-5.17611100	-0.90623700
H	7.87494700	-5.05859200	-1.00842600
H	6.61994400	-5.83308200	-0.04547200
H	6.42459600	-5.69309400	-1.79783700
C	3.82549200	1.97326700	2.21320300
H	3.71375300	0.89834600	2.37444100
H	4.17546900	2.42725100	3.14579600
H	2.81981600	2.36157300	2.01429000
C	6.12998100	0.95673000	-2.23909200
H	6.50006100	-0.03821200	-1.97558700
H	5.21212800	0.80786200	-2.81853000
H	6.86309300	1.43146400	-2.89783900
C	7.20191300	5.12913100	0.30357000
H	8.26552800	4.97445600	0.09291600
H	6.83810800	5.87303200	-0.41565800
H	7.11618100	5.56729700	1.30198700
C	-3.86039600	1.19230300	-0.82131400
C	-4.67559700	0.36768900	-0.02200900
C	-2.47271600	1.16396400	-0.77900600
H	-4.33720400	1.81656700	-1.57189600
C	-4.00241800	-0.44546600	0.94937400
C	-1.76115100	0.30474000	0.08364800
H	-1.91448200	1.76038900	-1.49265700
C	-2.55220000	-0.46990300	1.00090200
C	-4.55666200	-1.18756800	1.98015900
C	-2.09084000	-1.21433700	2.07402100
H	-5.60180900	-1.30156600	2.22900700
H	-1.06562700	-1.34297100	2.38983700
S	-3.36423500	-1.89844200	2.99110300
7			
C	1.85492700	-1.07085400	0.17335200
C	0.47145800	-1.10287500	0.21716500
C	-0.28299500	0.06617200	-0.01986100
C	0.42860800	1.26401400	-0.25778200
C	1.80995500	1.28862100	-0.25992800

C	2.57305700	0.11884400	-0.06054100
H	2.40853100	-1.99328900	0.32988900
H	-0.05183000	-2.02664400	0.42999600
H	-0.11630600	2.19283500	-0.39497500
H	2.32635200	2.23230000	-0.41724400
C	-6.08997400	0.29774200	-0.21016400
C	-6.96050700	-0.78597000	0.05786400
C	-6.70027100	1.52583500	-0.56186100
C	-8.32781500	-0.66147200	-0.04802500
H	-6.52310600	-1.72615700	0.37154600
C	-8.06497600	1.66646300	-0.66663900
H	-6.08279900	2.40181000	-0.72767000
C	-8.92654500	0.56736200	-0.41978900
H	-8.94476900	-1.52571000	0.16761300
H	-8.47300200	2.63449900	-0.93176700
N	-10.28112900	0.69308800	-0.52805900
C	-11.14231400	-0.44151300	-0.27181500
H	-12.17883200	-0.15084900	-0.43848900
H	-10.90923000	-1.27678900	-0.94251200
H	-11.04637700	-0.79377200	0.76268200
C	-10.87270100	1.96782600	-0.87179800
H	-11.95605300	1.86218600	-0.91285700
H	-10.63188000	2.73626400	-0.12686200
H	-10.52691300	2.31799100	-1.85196500
B	4.13892000	0.14491100	-0.09212400
C	4.92008600	-1.21030600	-0.32163800
C	5.84521700	-1.67586900	0.64900900
C	4.69772600	-2.01674900	-1.46034100
C	6.48249200	-2.90100100	0.47831000
C	5.37034100	-3.23452100	-1.60339800
C	6.26024500	-3.70107000	-0.64435000
H	7.17450600	-3.24470200	1.24547700
H	5.18886200	-3.83203900	-2.49562300
C	4.88158700	1.52797700	0.10150800
C	5.73613200	2.02765000	-0.91553900
C	4.68630900	2.32687000	1.25020200
C	6.33347700	3.27686200	-0.77757000
C	5.31645100	3.57097200	1.35823600
C	6.14009500	4.06849200	0.35646400
H	6.96889500	3.64704100	-1.58058900
H	5.15484200	4.16421100	2.25714900
C	3.80966600	-1.59028300	-2.60215800
H	4.41626600	-1.28701300	-3.46447100
H	3.17276300	-2.41690300	-2.93336600
H	3.15959100	-0.75318200	-2.34378700
C	6.13523600	-0.89167800	1.90249100
H	6.87972000	-1.40483100	2.51725700
H	6.51297700	0.10912100	1.67329100
H	5.23619500	-0.76379600	2.51580000
C	6.95330300	-5.02568000	-0.79398500
H	8.02708600	-4.93855500	-0.59784000
H	6.55600500	-5.76132400	-0.08476900
H	6.82470900	-5.43310500	-1.80029000
C	3.87338500	1.86621300	2.43351900
H	3.23126900	1.01529600	2.20124100
H	4.53403500	1.56842700	3.25701200
H	3.23625400	2.67266700	2.81073900
C	5.98958500	1.25265300	-2.18262100
H	6.42143800	0.26967800	-1.97281200
H	5.06444600	1.08254900	-2.74468400
H	6.67637800	1.79462500	-2.83850300
C	6.81460500	5.40497800	0.48562500
H	7.89888200	5.29192700	0.60127500
H	6.65006500	6.02211300	-0.40400900
H	6.44404600	5.95736900	1.35322000
C	-3.81945900	1.08906300	-0.82177800
C	-4.63546300	0.17086800	-0.13399100

C	-2.43520100	1.03608700	-0.78566600
H	-4.28287300	1.84209900	-1.45094200
C	-3.97747700	-0.86109100	0.59318000
C	-1.74234800	0.06006100	-0.04664400
H	-1.87384000	1.74186700	-1.38686200
C	-2.54073800	-0.91554500	0.64622400
S	-3.37233200	-2.73503100	1.98555400
N	-2.05351500	-1.90727800	1.40499700
N	-4.59314900	-1.83197700	1.30147000

8

C	1.85241600	-1.06198100	0.29462700
C	0.47600100	-1.07747900	0.36069600
C	-0.28431600	0.09359200	0.09854100
C	0.44934400	1.27551100	-0.19800900
C	1.82482700	1.28012000	-0.23095900
C	2.59874600	0.10929100	-0.00420200
H	2.39691300	-1.98424900	0.48500700
H	-0.04046600	-1.99861100	0.60025600
H	-0.07901800	2.21153900	-0.35671400
H	2.34558300	2.21009900	-0.44791800
C	-6.08897700	0.29539700	-0.21534600
C	-6.92978400	-0.84212100	-0.21315000
C	-6.72371900	1.54871000	-0.39388500
C	-8.29480400	-0.74318500	-0.36044100
H	-6.48810900	-1.82970300	-0.13720200
C	-8.08600800	1.66654600	-0.53936300
H	-6.12209600	2.45119400	-0.37419700
C	-8.92079400	0.51905800	-0.52212900
H	-8.88467400	-1.65168600	-0.37443500
H	-8.51660300	2.65457700	-0.64874900
N	-10.27248000	0.62603300	-0.66188600
C	-11.10908900	-0.55487800	-0.61386200
H	-12.15434200	-0.25756400	-0.68470400
H	-10.88949000	-1.23723500	-1.44432800
H	-10.97158000	-1.09907500	0.32737800
C	-10.88634400	1.92031500	-0.87278100
H	-11.96076600	1.79240800	-0.99573400
H	-10.71646600	2.58781300	-0.01926000
H	-10.49401400	2.40431600	-1.77479100
B	4.14605700	0.11307000	-0.08096200
C	4.91932900	-1.25894500	-0.27141700
C	5.95719800	-1.64986800	0.61573600
C	4.61440000	-2.14038300	-1.33966800
C	6.61975800	-2.86331500	0.44284500
C	5.31188800	-3.34136400	-1.49030800
C	6.31318700	-3.73033100	-0.60619700
H	7.40256100	-3.14041600	1.14786400
H	5.06883900	-3.98875200	-2.33220900
C	4.92811100	1.49054000	0.02436800
C	5.85708300	1.88599700	-0.97501100
C	4.73402700	2.37464800	1.11454800
C	6.51855400	3.10829800	-0.88453700
C	5.42891300	3.58571400	1.17966900
C	6.32155300	3.97879400	0.18846200
H	7.21182400	3.39138000	-1.67571700
H	5.26988800	4.23757000	2.03791100
C	3.56049100	-1.82280900	-2.37065300
H	3.78299700	-2.32493700	-3.31768000
H	2.56711200	-2.15301900	-2.04517100
H	3.47866800	-0.74946500	-2.55910500
C	6.35608800	-0.78989100	1.78682300
H	7.13299800	-1.27936600	2.38169200
H	6.73363900	0.18516100	1.46540700
H	5.50459500	-0.59435800	2.44790000
C	7.03072700	-5.04132600	-0.76277400
H	8.10127600	-4.94020400	-0.55640600

H	6.63966200	-5.79480700	-0.06761400
H	6.91722200	-5.44049900	-1.77488000
C	3.80355500	2.04908900	2.25571400
H	3.76827000	0.97667300	2.46349400
H	4.11397500	2.56838300	3.16808300
H	2.77334800	2.35255300	2.03599200
C	6.13698100	1.01999700	-2.17582500
H	6.58970200	0.06591400	-1.89006000
H	5.21823600	0.77924100	-2.72134800
H	6.81440300	1.52576700	-2.87039000
C	7.06147200	5.28448500	0.26863800
H	8.14486800	5.12786000	0.32995700
H	6.87870000	5.90258100	-0.61788100
H	6.75880500	5.86178300	1.14683200
C	-3.80777900	1.14720400	-0.72016700
C	-4.64590900	0.20878100	-0.06749200
C	-2.43516600	1.08969400	-0.65812600
H	-4.26664500	1.89675400	-1.35828000
C	-3.97055800	-0.77539500	0.68638200
C	-1.72967500	0.10792400	0.08720000
H	-1.86456400	1.79570600	-1.24961600
C	-2.55911100	-0.82867600	0.79144400
N	-2.08359600	-1.79212800	1.64436600
C	-3.03930600	-2.47247400	2.18178000
H	-2.89264100	-3.28475700	2.88357500
S	-4.65564000	-1.99406000	1.72209100

Table S3 The fluorescence (λ_{fl}) wavelengths (in nm), the oscillator strength f , main assignments (coefficient), and main electronic transitions of **5** at the TD-PBE0/6-31+G(d,p)//TD-PBE0/6-31(d,p) level and discussion.

Electronic transition	λ_{fl}	f	Assignment
$S_1 \rightarrow S_0$	615	0.00	L \rightarrow H (0.70)
$S_2 \rightarrow S_0$	361	0.08	L-2 \rightarrow H (0.70)
$S_3 \rightarrow S_0$	361	0.18	L-3 \rightarrow H (0.68)
			L-1 \rightarrow H (0.12)

For the DMPB fragments serve as acceptors for the designed compounds, the twist angles between DMPB with CB are the important parameter for molecular π -conjugation. The twist angles between DMPB with CB in S_0 for **1–8** are 1.0°, 35.2°, -18.8°, 3.2°, 17.2°, 44.0°, 34.4°, and 36.9°, while the corresponding values in S_1 are -0.6°, 25.0°, -2.2°, 0.2°, -88.7°, 33.5°, 22.7°, and 22.9°, respectively. It reveals clearly that the twist angles between DMPB with CB in S_1 are smaller than those in S_0 for the designed compounds except for **5**. The conjugative effects of **1–4** and **6–8** in S_1 become higher than those in S_0 , because the twist angles between DMPB with CB decrease. As a consequence, the electron can move more fluently from the donors to the acceptors. Therefore, their λ_{abs} values are larger than those λ_{fl} values for **1–4** and **6–8**. On the contrary, the twist angle between DMPB with CB of **5** in S_0 is larger than that in S_1 (the deviation is 71.5°). It suggests that the conjugative effect between DMPB, CB, and MBA fragments in **5** is weaker than that in S_0 . This worse conjugative effect weakens the ICT character of **5**, resulting in the λ_{fl} value of **5** is smaller than that of λ_{abs} value.

Table S4 The calculated total energies (in kcal/mol) of the compounds under investigation in different space groups.

Space groups	1	2	3	4	5	6	7	8
C_2	173.73016131	200.00623688	178.25653316	185.93494506	190.99359068	208.63427948	206.45774221	198.06819033
C_2/c	177.04881310	199.57291521	180.68453671	187.77089431	188.92594770	213.52349089	211.64571780	203.96698905
C_c	177.04881310	196.39055637	180.58637673	184.53175093	190.59844137	212.89667199	203.71115529	203.25751180
$P2_1$	176.90848167	192.53221631	175.79397230	180.84396990	185.03055869	202.08844942	209.31644185	199.60067521

<i>P2₁/c</i>	176.42410707	195.55836105	178.43460011	185.35248615	188.84496553	210.61724387	210.11741969	200.43507507
<i>P2₁2₁2₁</i>	177.80224786	195.88934875	179.46967553	184.04741351	191.92150542	205.88271607	206.73557997	198.56399752
<i>P$\bar{1}$</i>	176.16306638	198.23601554	178.91793038	187.51077622	189.38895563	213.74479998	207.34022744	206.42429608
<i>Pbca</i>	174.64529770	195.77756116	181.26127922	185.22009682	190.40887938	208.89126789	209.90127566	202.79585780
<i>Pbcn</i>	178.49861691	198.79087432	182.08143352	187.45865951	193.16858719	209.48374108	211.77544258	208.77768459
<i>Pna2₁</i>	177.76143847	197.12457580	182.64566694	186.63833462	187.47448840	205.71774890	209.50422385	204.97166147

Table S5 The calculated crystal cell parameters of the compounds under investigation with the lowest total energies.

Species	Space groups	a (Å)	b (Å)	c (Å)	α (deg)	β (deg)	γ (deg)
1	<i>C2</i>	31.12	15.13	13.45	90.00	75.83	90.00
2	<i>P2₁</i>	16.21	20.26	10.51	90.00	115.49	90.00
3	<i>P2₁</i>	16.65	13.21	15.76	90.00	111.25	90.00
4	<i>P2₁</i>	14.40	16.92	12.91	90.00	83.69	90.00
5	<i>P2₁</i>	15.10	16.45	14.42	90.00	117.89	90.00
6	<i>P2₁</i>	21.98	16.66	9.17	90.00	66.64	90.00
7	<i>C2</i>	41.64	12.00	29.82	90.00	147.04	90.00
8	<i>C2</i>	45.71	10.28	44.42	90.00	162.27	90.00

Table S6 Center-center distance and the corresponding hole and electron coupling (eV) between the dimer in all of the nearest neighbor pathways for **1–6** in different space groups.

Species	space group	Pathway	Distance (Å)	Electron coupling	Hole coupling
1	<i>C2</i>	1	13.450	-2.25×10^{-4}	7.08×10^{-7}
		2	13.450	-2.25×10^{-4}	7.08×10^{-7}
		3	15.133	-4.71×10^{-5}	-1.36×10^{-5}
		4	15.133	-4.71×10^{-5}	-1.36×10^{-5}
		5	7.401	-9.41×10^{-4}	-1.33×10^{-4}
		6	17.786	2.35×10^{-8}	3.49×10^{-9}
		7	17.786	2.35×10^{-8}	3.49×10^{-9}
		8	11.039	-4.27×10^{-4}	3.75×10^{-4}
		9	11.039	-4.27×10^{-4}	3.75×10^{-4}
2	<i>P2₁</i>	Pathway	Distance (Å)	Electron coupling	Hole coupling
		1	10.512	-3.08×10^{-5}	-3.38×10^{-6}
		2	10.512	-3.08×10^{-5}	-3.38×10^{-6}
		3	15.053	-1.43×10^{-6}	5.40×10^{-7}
		4	15.053	-1.43×10^{-6}	5.40×10^{-7}
		5	10.911	-8.02×10^{-5}	-4.93×10^{-5}
		6	10.911	-3.29×10^{-4}	-4.48×10^{-5}
		7	10.911	-8.02×10^{-5}	-4.93×10^{-5}
8	10.911	-3.29×10^{-4}	-4.48×10^{-5}		
3	<i>P2₁</i>	Pathway	Distance (Å)	Electron coupling	Hole coupling
		1	15.762	-2.30×10^{-4}	5.27×10^{-5}
		2	15.762	-2.30×10^{-4}	5.27×10^{-5}
		3	16.648	-7.42×10^{-5}	-9.39×10^{-5}
4	16.648	-7.42×10^{-5}	-9.39×10^{-5}		

			5	14.215	-2.44×10^{-7}	-8.45×10^{-8}
			6	10.487	9.03×10^{-4}	1.85×10^{-4}
			7	14.215	-2.44×10^{-7}	-8.45×10^{-8}
			8	10.487	9.03×10^{-4}	1.85×10^{-4}
4	$P2_I$	Pathway	Distance (Å)	Electron coupling	Hole coupling	
			1	12.906	3.26×10^{-14}	2.45×10^{-15}
			2	12.906	3.26×10^{-14}	2.45×10^{-15}
			3	14.396	3.63×10^{-5}	7.77×10^{-5}
			4	14.396	3.63×10^{-5}	7.77×10^{-5}
			5	10.651	4.35×10^{-4}	-8.02×10^{-4}
			6	10.651	4.35×10^{-4}	-8.02×10^{-4}
			7	18.984	2.81×10^{-4}	-3.02×10^{-4}
			8	17.888	-6.08×10^{-7}	1.30×10^{-6}
5	$P2_I$	Pathway	Distance (Å)	Electron coupling	Hole coupling	
			1	15.101	4.84×10^{-4}	-6.59×10^{-4}
			2	15.101	4.84×10^{-4}	-6.59×10^{-4}
			3	14.422	1.75×10^{-16}	2.80×10^{-17}
			4	14.422	1.75×10^{-16}	2.80×10^{-17}
			5	10.718	-2.30×10^{-3}	1.22×10^{-4}
			6	14.449	-1.470×10^{-6}	2.24×10^{-8}
			7	10.718	-2.30×10^{-3}	1.22×10^{-4}
			8	14.449	-1.470×10^{-6}	2.24×10^{-8}
6	$P2_I$	Pathway	Distance (Å)	Electron coupling	Hole coupling	
			1	9.171	-4.50×10^{-3}	-4.37×10^{-4}
			2	9.171	-4.50×10^{-3}	-4.37×10^{-4}
			3	20.180	2.10×10^{-4}	7.02×10^{-6}
			4	20.180	2.10×10^{-4}	7.02×10^{-6}
			5	10.987	8.99×10^{-4}	-3.58×10^{-4}
			6	10.987	8.99×10^{-4}	-3.58×10^{-4}