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局域和长程杂化密度泛函研究推拉结构有机发光分子

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Local and Long-Range Hybrid Density Functional Study on an Organic Light-Emitting Molecule with Pull-Push Structure

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Supporting Information

Table 1 Relative energy (in eV) and dipole moment (in Debye) for the four isomers of DCDCC in gas phase.

	Cis1	Cis2	Trans1	Trans2
Energy	0.0978	0.0975	0.0004	0
Dipole moment	8.22	8.19	8.53	8.53

Table2 Bond length (in Å) and dihedral angle (in º) of the minimum S_0 and S_1 geometries in hexane and DMF solvents optimized by different methods.

Hexane B3LYP	S_0	S_1
N11-C22	1.414	1.447
C22-C27	1.405	1.399
C27-C26	1.387	1.387
C26-C25	1.411	1.422
C25-C32	1.459	1.442
C32-C33	1.357	1.383
C33-C38	1.445	1.413
C38-C39	1.372	1.404
C39-C40	1.431	1.397
C40-C55	1.385	1.423
C55-C56	1.428	1.416
C12-N11-C22-C27	-50.9	90.1
C4-N11-C22-C23	-51.0	89.8
C26-C25-C32-C33	0.0	-1.6
C25-C32-C33-C38	-178.9	179.6
C32-C33-C38-C39	177.2	177.6
C39-C40-C55-C56	-179.4	-179.8

DMF B3LYP	S_0	S_1
N11-C22	1.417	1.416
C22-C27	1.405	1.408
C27-C26	1.388	1.382
C26-C25	1.411	1.424
C25-C32	1.458	1.438
C32-C33	1.358	1.386
C33-C38	1.444	1.414
C38-C39	1.374	1.407
C39-C40	1.427	1.397
C40-C55	1.390	1.428
C55-C56	1.426	1.414
C12-N11-C22-C27	-51.6	-50.4
C4-N11-C22-C23	-51.7	-50.6
C26-C25-C32-C33	0.0	-0.2
C25-C32-C33-C38	-178.7	-179.7
C32-C33-C38-C39	177.0	177.5
C39-C40-C55-C56	-179.4	-179.7

Hexane PBE0	S_0	S_1
N11-C22	1.406	1.436
C22-C27	1.401	1.396
C27-C26	1.384	1.382
C26-C25	1.406	1.419
C25-C32	1.454	1.435
C32-C33	1.354	1.381
C33-C38	1.442	1.408
C38-C39	1.368	1.400
C39-C40	1.428	1.393
C40-C55	1.380	1.417
C55-C56	1.424	1.412
C12-N11-C22-C27	-50.2	89.1
C4-N11-C22-C23	-50.4	88.8
C26-C25-C32-C33	0.6	-2.1
C25-C32-C33-C38	-178.6	179.6
C32-C33-C38-C39	176.9	177.3
C39-C40-C55-C56	-179.5	-180.0

DMF PBE0	S_0	S_1
N11-C22	1.409	1.397
C22-C27	1.401	1.409
C27-C26	1.384	1.376
C26-C25	1.407	1.424
C25-C32	1.454	1.425
C32-C33	1.355	1.389
C33-C38	1.441	1.407
C38-C39	1.370	1.406
C39-C40	1.424	1.393
C40-C55	1.385	1.422
C55-C56	1.422	1.410
C12-N11-C22-C27	-50.7	-45.9
C4-N11-C22-C23	-50.9	-46.0
C26-C25-C32-C33	0.7	-0.5
C25-C32-C33-C38	-178.5	-179.5
C32-C33-C38-C39	176.8	177.3

C39-C40-C55-C56	-179.4	-180.0

Hexane BMK	S_0	S_1
N11-C22	1.410	1.397
C22-C27	1.408	1.418
C27-C26	1.392	1.382
C26-C25	1.412	1.434
C25-C32	1.469	1.432
C32-C33	1.355	1.396
C33-C38	1.459	1.416
C38-C39	1.368	1.409
C39-C40	1.444	1.408
C40-C55	1.380	1.418
C55-C56	1.437	1.425
C12-N11-C22-C27	-49.1	-45.4
C4-N11-C22-C23	-50.0	-45.7
C26-C25-C32-C33	-0.2	-1.3
C25-C32-C33-C38	-178.5	-178.5
C32-C33-C38-C39	175.8	179.9
C39-C40-C55-C56	-179.0	-179.6

DMF BMK	S_0	S_1
N11-C22	1.413	1.388
C22-C27	1.408	1.423
C27-C26	1.393	1.379
C26-C25	1.413	1.438
C25-C32	1.469	1.420
C32-C33	1.356	1.408
C33-C38	1.458	1.406
C38-C39	1.371	1.422
C39-C40	1.440	1.399
C40-C55	1.384	1.430
C55-C56	1.435	1.422
C12-N11-C22-C27	-49.6	-41.5
C4-N11-C22-C23	-50.5	-41.8
C26-C25-C32-C33	-0.9	-1.0
C25-C32-C33-C38	-178.2	-178.4
C32-C33-C38-C39	175.2	176.6
C39-C40-C55-C56	-179.0	-179.6

Hexane BHLYP	S_0	S_1
N11-C22	1.407	1.387
C22-C27	1.393	1.406
C27-C26	1.379	1.367
C26-C25	1.398	1.423
C25-C32	1.458	1.411
C32-C33	1.341	1.390
C33-C38	1.447	1.397
C38-C39	1.353	1.401
C39-C40	1.433	1.393
C40-C55	1.365	1.405
C55-C56	1.426	1.413
C12-N11-C22-C27	-53.8	-43.9
C4-N11-C22-C23	-53. 8	-44.0
C26-C25-C32-C33	1.57	-0.1
C25-C32-C33-C38	-178.9	-179.9
C32-C33-C38-C39	177.0	177.7
C39-C40-C55-C56	-179.3	-180.0

DMF BHLYP	S_0	S_1
N11-C22	1.410	1.384
C22-C27	1.393	1.408
C27-C26	1.379	1.365
C26-C25	1.399	1.425
C25-C32	1.458	1.403
C32-C33	1.341	1.399
C33-C38	1.446	1.388
C38-C39	1.356	1.412
C39-C40	1.428	1.385
C40-C55	1.370	1.415
C55-C56	1.423	1.409
C12-N11-C22-C27	-54.4	-42.5
C4-N11-C22-C23	-54.5	-42.3
C26-C25-C32-C33	1.3	0.4
C25-C32-C33-C38	-178.6	-179.9
C32-C33-C38-C39	176.7	178.1
C39-C40-C55-C56	-179.1	-180.0

Hexane CAM-B3LYP	S_0	S_1
N11-C22	1.412	1.390
C22-C27	1.397	1.411
C27-C26	1.384	1.371
C26-C25	1.402	1.427
C25-C32	1.463	1.413
C32-C33	1.344	1.395
C33-C38	1.453	1.401
C38-C39	1.357	1.407
C39-C40	1.438	1.397
C40-C55	1.369	1.411
C55-C56	1.430	1.416
C12-N11-C22-C27	-52.8	-42.9
C4-N11-C22-C23	-52.8	-43. 0
C26-C25-C32-C33	1.7	0.1
C25-C32-C33-C38	-178.8	-179.9
C32-C33-C38-C39	176.8	177.8
C39-C40-C55-C56	-179.3	179.9

Hexane ωB97XD	S_0	S_1
N11-C22	1.411	1.390
C22-C27	1.398	1.411
C27-C26	1.385	1.373
C26-C25	1.403	1.429
C25-C32	1.466	1.413
C32-C33	1.345	1.399
C33-C38	1.455	1.399
C38-C39	1.358	1.412
C39-C40	1.441	1.397
C40-C55	1.370	1.413
C55-C56	1.431	1.417
C12-N11-C22-C27	-53.6	-44.6
C4-N11-C22-C23	-52.6	-43.9
C26-C25-C32-C33	3.9	1.2
C25-C32-C33-C38	-179.5	179.4
C32-C33-C38-C39	176.3	178.8
C39-C40-C55-C56	-179.5	179.8

DMF CAM-B3LYP	S_0	S_1
N11-C22	1.415	1.388
C22-C27	1.397	1.413
C27-C26	1.384	1.369
C26-C25	1.402	1.429
C25-C32	1.463	1.405
C32-C33	1.345	1.404
C33-C38	1.452	1.391
C38-C39	1.359	1.418
C39-C40	1.434	1.388
C40-C55	1.373	1.422
C55-C56	1.428	1.413
C12-N11-C22-C27	-53.4	-41.8
C4-N11-C22-C23	-53.6	-41.5
C26-C25-C32-C33	1.34	0.5
C25-C32-C33-C38	-178.6	-179.8
C32-C33-C38-C39	176.5	178.2
C39-C40-C55-C56	-179.2	179.8

DMF ωB97XD	S_0	S_1
N11-C22	1.414	1.389
C22-C27	1.398	1.412
C27-C26	1.386	1.371
C26-C25	1.404	1.431
C25-C32	1.466	1.406
C32-C33	1.346	1.408
C33-C38	1.454	1.390
C38-C39	1.361	1.423
C39-C40	1.436	1.389
C40-C55	1.375	1.424
C55-C56	1.429	1.414
C12-N11-C22-C27	-54.2	-43.7
C4-N11-C22-C23	-53.1	-42.9
C26-C25-C32-C33	3.3	1.8
C25-C32-C33-C38	-179.5	-179.9
C32-C33-C38-C39	176.4	179.3
C39-C40-C55-C56	-179.4	179.8

Hexane M062X	S_0	S_1
N11-C22	1.411	1.389
C22-C27	1.400	1.413
C27-C26	1.385	1.373
C26-C25	1.404	1.429
C25-C32	1.464	1.416
C32-C33	1.347	1.395
C33-C38	1.454	1.404
C38-C39	1.359	1.406
C39-C40	1.441	1.400
C40-C55	1.369	1.409
C55-C56	1.433	1.419
C12-N11-C22-C27	-49.9	-42. 5
C4-N11-C22-C23	-50.4	-42.6
C26-C25-C32-C33	3.2	0.0
C25-C32-C33-C38	-178.6	179.9
C32-C33-C38-C39	175.8	177.2
C39-C40-C55-C56	-179.2	-179. 9

DMF M062X	S_0	S_1
N11-C22	1.413	1.385
C22-C27	1.400	1.415
C27-C26	1.386	1.371
C26-C25	1.405	1.431
C25-C32	1.464	1.408
C32-C33	1.348	1.405
C33-C38	1.453	1.394
C38-C39	1.361	1.419
C39-C40	1.438	1.391
C40-C55	1.372	1.421
C55-C56	1.431	1.415
C12-N11-C22-C27	-50. 3	-40.9
C4-N11-C22-C23	-50.7	-40.7
C26-C25-C32-C33	3.1	0.8
C25-C32-C33-C38	-178.4	-180.0
C32-C33-C38-C39	175.7	177.8
C39-C40-C55-C56	-179.1	-180.0

Hexane M06	S_0	S_1
N11-C22	1.407	1.426
C22-C27	1.400	1.398
C27-C26	1.382	1.380
C26-C25	1.405	1.417
C25-C32	1.452	1.436
C32-C33	1.351	1.377
C33-C38	1.440	1.410
C38-C39	1.366	1.396
C39-C40	1.428	1.397
C40-C55	1.378	1.412
C55-C56	1.425	1.414
C12-N11-C22-C27	-48.9	-58.3
C4-N11-C22-C23	-49.0	-58.8
C26-C25-C32-C33	-1.4	2.0
C25-C32-C33-C38	-178.2	-179.8
C32-C33-C38-C39	176.0	178.0
C39-C40-C55-C56	-179.1	-179.5

DMF M06	S_0	S_1
N11-C22	1.409	1.395
C22-C27	1.400	1.409
C27-C26	1.383	1.373
C26-C25	1.405	1.424
C25-C32	1.452	1.419
C32-C33	1.352	1.390
C33-C38	1.439	1.402
C38-C39	1.369	1.407
C39-C40	1.423	1.392
C40-C55	1.383	1.420
C55-C56	1.423	1.411
C12-N11-C22-C27	-49.1	-44.0
C4-N11-C22-C23	-49.6	-44.2
C26-C25-C32-C33	-1.6	1.0
C25-C32-C33-C38	-177.8	178.9
C32-C33-C38-C39	175.5	178.1
C39-C40-C55-C56	-179.0	-179.7