

Supporting Information

Thermally activated delayed fluorescence materials with aggregation-induced emission properties: A QM/MM study

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We use the Forcite module with the Universal force field¹ in the Materials Studio software to predict the amorphous configurations of DMAC-CNQ. The ensemble of dynamics is NVT, and the initial velocity is chosen randomly. We perform the MD simulations for DMAC-CNQ in the amorphous phase: (1) the initial configuration is constructed by randomly placing 25 molecules in a box ($28.2 \times 28.2 \times 28.2$ Å); (2) perform 5 ns simulation at 600 K, then cool down from 600 K to 298 K gradually within 3 ns. Four representative amorphous configurations are generated as shown in Fig. S1.

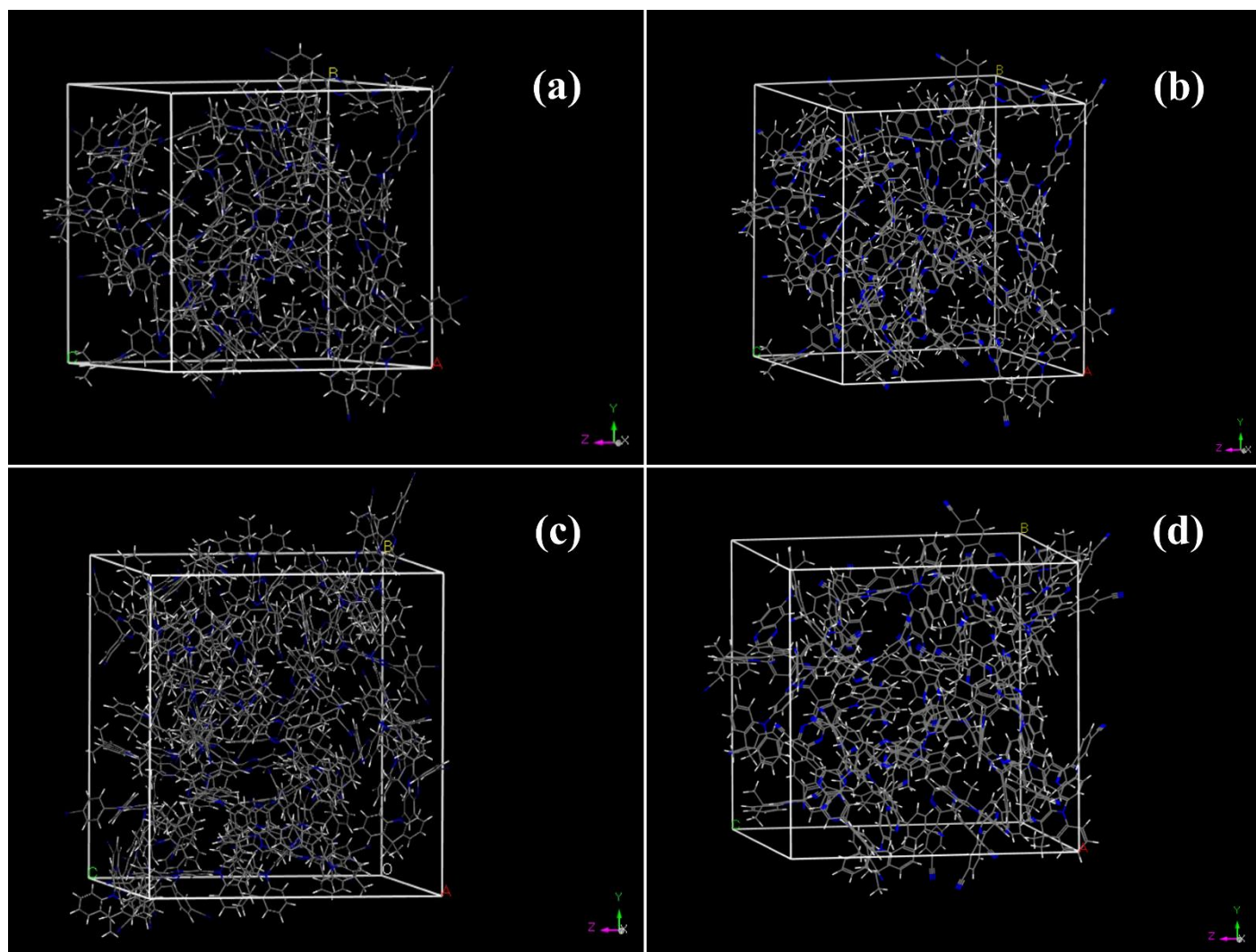


Figure S1. Four amorphous configurations of DMAC-CNQ, (a) for amorphous-1, (b) for amorphous-2, (c) for amorphous-3, and (d) for amorphous-4.

Table S1. Calculated the vertical excited state energies (in eV) and vertical singlet-triplet gaps ΔE_{ST^*} at the BMK/6-31G* level.

	gas	crystal	amorphous
E(T ₁)	2.73	2.72	2.66
E(S ₁)	2.81	2.80	3.04
E(T ₂)	2.85	2.88	3.13
E(T ₃)	3.17	3.17	3.17
E(T ₄)	3.19	3.24	3.54
E(T ₅)	3.41	3.45	3.56
E(T ₆)	3.45	3.49	3.59
E(S ₂)	3.45	3.50	3.69
ΔE_{ST^*}	0.08 (0.09 exp.)	0.08	0.38

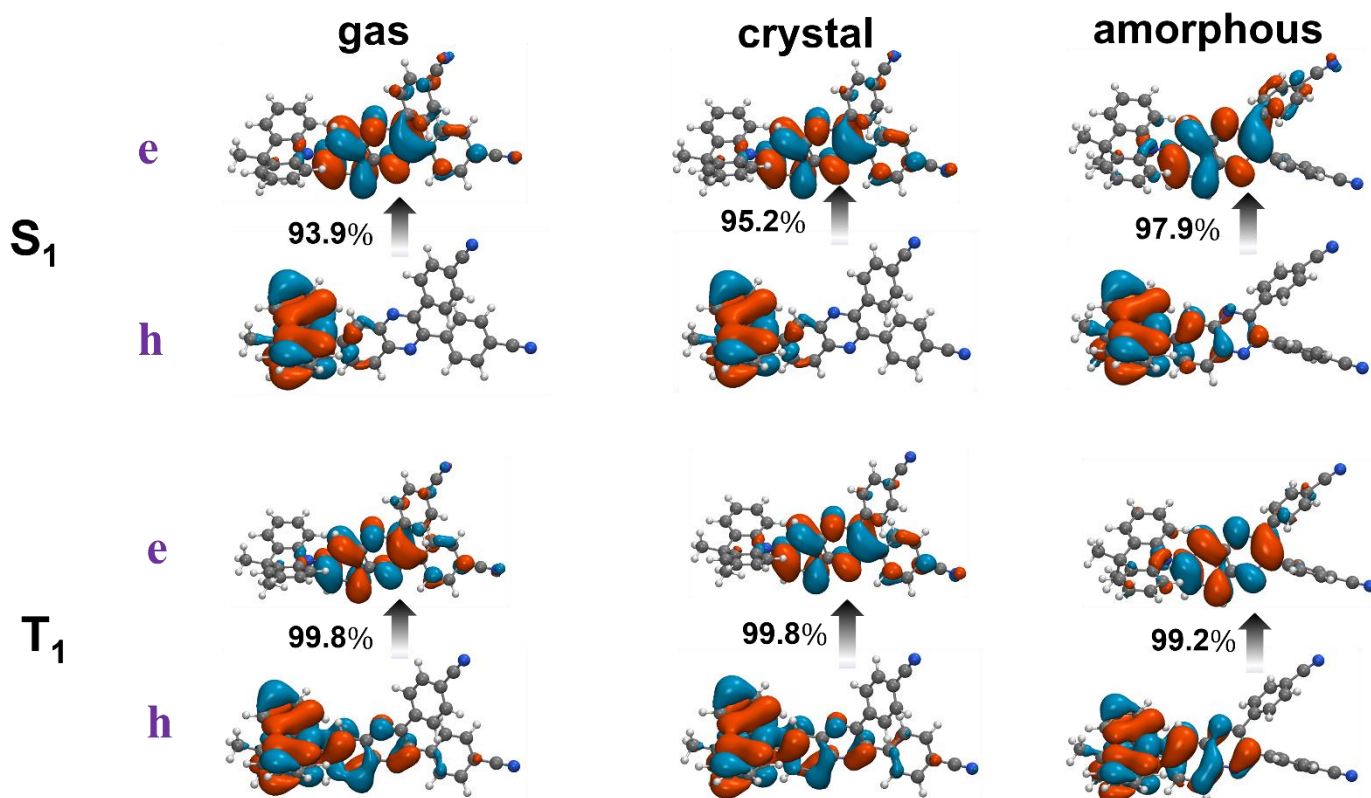


Figure S2. Natural transition orbitals (NTO) for the S_1 and T_1 states of DMAC-CNQ in gas, crystal and amorphous phases at the BMK/6-31G* level, respectively the Eigenvalue of NTOs (isovalue = 0.02). The proportions of HONTO-LUNTO transition for the S_1 and T_1 state are listed.

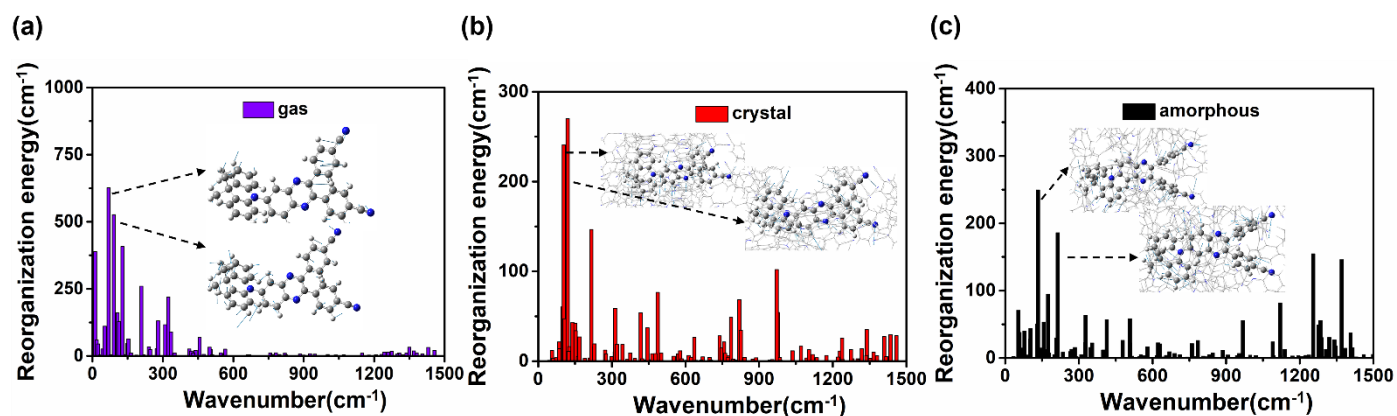


Figure S3. Calculated reorganization energies (a-c) at the BMK/6-31G* level for the conversion between T_1 and S_1 , and two key vibration modes for DMAC-CNQ in gas, crystal, and amorphous states, respectively.

Coordinates (unit: Å)

DMAC-CNQ (gas)- S_0

N	-1.72527500	-1.92013000	-0.26308100
N	3.65125700	-0.37920700	-0.00230700
N	-1.06190300	0.77787100	0.07850000
C	-0.42691900	-1.52975400	-0.23959300
C	1.27767200	0.22440700	0.07432400
N	-9.01692200	-3.66786500	0.38688500
C	-2.66473900	-1.01101800	-0.11387100
C	-4.06211800	-1.53899100	-0.01391700

C	-0.08833800	-0.16268800	-0.01076300
C	2.26800800	-0.72878700	-0.06902200
C	4.30257500	0.00847200	-1.19505500
C	-4.43358100	-2.63560300	-0.81336100
C	-6.26045700	-1.56975700	1.02789900
C	-5.71061700	-3.18536000	-0.71561400
C	-6.62911500	-2.65030500	0.20601500
C	6.33042300	0.64578200	-2.34679700
C	5.70781200	0.17863500	-1.18198900
C	4.23047400	0.67994600	-3.53206500
C	3.57582300	0.24567200	-2.37679500
C	0.61086200	-2.49037600	-0.40424600
C	4.23861900	-0.05708000	1.24192200
C	-2.31887800	0.40005900	-0.00699800
C	5.60885100	0.89940000	-3.51902700
C	5.64312600	0.11741700	1.30183100
C	1.92761000	-2.09305100	-0.32016200
C	-4.98477300	-1.01842100	0.91239500
C	3.46577000	0.08943900	2.40907300
C	-3.32225200	1.51130100	-0.03645500
C	6.47753900	-0.26023200	0.07025700
C	6.21337600	0.51748000	2.51732300
C	-7.95376200	-3.21464800	0.30920500

C	4.06893600	0.45747200	3.61442000
C	-4.42119200	1.49378100	-0.91500000
C	-3.11149800	2.63766300	0.77938300
C	5.44300900	0.69540500	3.67180900
C	-5.30367900	2.57202500	-0.96691900
C	6.59870600	-1.81608800	0.03618800
C	-3.99466500	3.71532000	0.74489700
C	7.90258700	0.32750800	0.12021600
C	-5.09656900	3.68264000	-0.12896700
N	-6.75706900	5.68470900	-0.19865200
C	-6.01673900	4.79430900	-0.16930200
H	1.52030200	1.27169000	0.24106300
H	-3.70626000	-3.05395500	-1.50417700
H	-6.97071600	-1.17254900	1.74886400
H	-6.00225300	-4.02485000	-1.34203100
H	7.40516400	0.80402400	-2.35249800
H	3.64950400	0.86015700	-4.43461800
H	2.49956100	0.10701400	-2.39182800
H	0.33004600	-3.52613000	-0.58028300
H	6.12409900	1.25244300	-4.40969000
H	2.73881500	-2.80813700	-0.43803600
H	-4.70371400	-0.18514900	1.55151400
H	2.39406300	-0.07605400	2.37997300

H	7.28641100	0.67826600	2.57299700
H	3.45082700	0.56890500	4.50330900
H	-4.58071000	0.64107900	-1.57016200
H	-2.24328800	2.65935500	1.43282400
H	5.91683900	0.99827700	4.60298800
H	-6.14854600	2.56250600	-1.65118500
H	5.60766100	-2.28451700	0.00750700
H	7.12411800	-2.17174500	0.93268400
H	7.15794300	-2.13041900	-0.85531300
H	-3.83863700	4.58113500	1.38381500
H	8.47887000	0.00512400	-0.75462700
H	8.43875500	-0.04073100	1.00224900
H	7.88921400	1.42477900	0.14782400

DMAC-CNQ (gas)-S₁

N	-1.76974600	-1.82781300	-0.60636900
N	3.62954600	-0.40313000	-0.11420000
N	-1.06081800	0.77764800	0.22866800
C	-0.47676500	-1.46004000	-0.52956000
C	1.25816100	0.17863500	0.10797300
N	-9.04085300	-3.69584600	-0.13760100
C	-2.71225400	-0.91544600	-0.26319200

C	-4.10066900	-1.45843700	-0.23496700
C	-0.11274900	-0.14734700	-0.04400300
C	2.23151300	-0.76732100	-0.25533100
C	4.26131200	0.22608500	-1.17057800
C	-4.45976000	-2.46494400	-1.15688500
C	-6.31929800	-1.64287600	0.76801700
C	-5.72925200	-3.03650300	-1.14063300
C	-6.67074700	-2.62510600	-0.17798400
C	6.21284000	1.22984700	-2.18899700
C	5.63414400	0.60390800	-1.08090700
C	4.13208900	1.11916500	-3.43260100
C	3.52137700	0.49419100	-2.35974100
C	0.55406300	-2.37270100	-0.89782800
C	4.27656900	-0.68270000	1.07519600
C	-2.35337600	0.41246300	0.07957200
C	5.48564200	1.48996100	-3.35446200
C	5.64993300	-0.34103700	1.25640700
C	1.90235500	-2.02836000	-0.76022600
C	-5.04862800	-1.07368300	0.73766100
C	3.55406800	-1.32177200	2.12543700
C	-3.31857700	1.54140400	0.23721800
C	6.46770100	0.35112100	0.17076100
C	6.24734100	-0.66108600	2.47938400

C	-7.98467200	-3.21794400	-0.15338900
C	4.18365500	-1.61866000	3.32166800
C	-4.45651700	1.68074700	-0.58377400
C	-3.03564000	2.55943500	1.17071600
C	5.53804300	-1.29144200	3.50593300
C	-5.30246000	2.78030800	-0.45815300
C	7.68689700	-0.54904000	-0.20071300
C	-3.87769400	3.65967200	1.31171600
C	6.98260000	1.71871300	0.71980100
C	-5.02022600	3.77493800	0.49748500
N	-6.58521500	5.83731200	0.75112200
C	-5.88970200	4.91711200	0.63534900
H	1.52417100	1.16519500	0.47856100
H	-3.71843600	-2.79288600	-1.87981800
H	-7.03929000	-1.34395400	1.52636200
H	-6.00027700	-3.80284400	-1.86344900
H	7.25811500	1.52549100	-2.14445300
H	3.55650400	1.32136700	-4.33209900
H	2.47804400	0.21000200	-2.40723500
H	0.25869100	-3.34966600	-1.27104300
H	5.97060900	1.98118200	-4.19491000
H	2.68717700	-2.73026900	-1.03555200
H	-4.78283400	-0.33180200	1.48594500

H	2.50996200	-1.56901300	1.98037500
H	7.29355100	-0.41089800	2.63789000
H	3.62190800	-2.10486700	4.11498500
H	-4.67263400	0.92510900	-1.33425500
H	-2.13655700	2.47098100	1.77401400
H	6.03757200	-1.52544400	4.44327000
H	-6.17434700	2.88248700	-1.09999600
H	7.35245700	-1.52164800	-0.58047400
H	8.31916600	-0.71696000	0.67858200
H	8.29820400	-0.06510900	-0.97109600
H	-3.65902500	4.43531300	2.04223300
H	7.59378200	2.22718400	-0.03474700
H	7.60200300	1.56474300	1.61090700
H	6.14320100	2.37154200	0.98642800

DMAC-CNQ (gas)-T₁

N	-1.77220800	-1.98164400	-0.05674400
N	3.61231400	-0.52759800	0.10464500
N	-1.04763300	0.75036800	-0.11368900
C	-0.49738700	-1.62767000	-0.06253300
C	1.24451600	0.10337200	0.09654100
N	-9.04708700	-3.45022900	1.21863300

C	-2.72210300	-0.98178100	-0.01797000
C	-4.09837300	-1.46329100	0.23252300
C	-0.10646600	-0.23035600	-0.01255700
C	2.26356400	-0.93358700	0.07175000
C	4.50138900	-0.84874500	-0.94681000
C	-4.44382500	-2.77658100	-0.16315300
C	-6.33389000	-1.20355800	1.18000500
C	-5.71508500	-3.28818600	0.07876600
C	-6.67168800	-2.50169500	0.74876100
C	6.67355900	-0.72247600	-1.99989100
C	5.83120200	-0.36403800	-0.93417800
C	4.90482100	-1.93459100	-3.09421900
C	4.04391800	-1.60116100	-2.05557200
C	0.54106700	-2.63000600	-0.09313500
C	4.03373200	0.24919300	1.19482400
C	-2.33658800	0.37505000	-0.16052500
C	6.23837100	-1.50941400	-3.06479700
C	5.31535000	0.85189000	1.21787600
C	1.88748100	-2.27980000	-0.03799900
C	-5.06360100	-0.69647100	0.92598400
C	3.17297500	0.38573600	2.31535800
C	-3.28178200	1.50391300	-0.43340400
C	6.36800200	0.58306900	0.14244100

C	5.63466000	1.67101500	2.30925200
C	-7.98813800	-3.02785600	1.00894800
C	3.52190100	1.20960700	3.38039400
C	-4.34087000	1.37764000	-1.35224200
C	-3.04940200	2.75452000	0.16887300
C	4.75108000	1.87747700	3.37223400
C	-5.16771400	2.46188600	-1.64129200
C	7.61382600	-0.06326000	0.81984800
C	-3.87422200	3.84423600	-0.10558500
C	6.78092300	1.92716700	-0.52783900
C	-4.94115400	3.69964400	-1.01128000
N	-6.48322600	5.72991700	-1.53003800
C	-5.79669100	4.82496900	-1.30094500
H	1.53250900	1.15148900	0.10117900
H	-3.68899500	-3.38006800	-0.65844700
H	-7.06626100	-0.60902600	1.72112000
H	-5.97709400	-4.29345700	-0.24321200
H	7.69888600	-0.35942300	-2.00052400
H	4.52687400	-2.51827500	-3.93067400
H	3.00730700	-1.91030000	-2.10640100
H	0.23076900	-3.67141100	-0.11471000
H	6.92229500	-1.76633500	-3.87062000
H	2.65521400	-3.05076600	-0.04133300

H	-4.80885900	0.29341700	1.29247500
H	2.24759100	-0.17804700	2.35044500
H	6.60999400	2.15224200	2.33464600
H	2.84280900	1.30914200	4.22407000
H	-4.51005500	0.42771200	-1.85286500
H	-2.20494500	2.85912000	0.84486200
H	5.03671500	2.52336500	4.19952600
H	-5.98315300	2.36089200	-2.35360900
H	7.34172200	-1.00839000	1.30516900
H	8.03557100	0.60644200	1.57850700
H	8.39648600	-0.26684900	0.07947500
H	-3.69805200	4.80650000	0.36960500
H	7.56229300	1.76068500	-1.27897600
H	7.17480600	2.62529200	0.22084300
H	5.92029600	2.39517900	-1.02092300

DMAC-CNQ (crystal)-S₀

N	-1.73683400	-1.86307300	-0.15692200
N	3.63335900	-0.34455000	0.03583700
N	-1.07370300	0.84692900	0.06004400
C	3.55120800	0.12312400	-2.37277600
H	2.47323900	0.02400300	-2.35453700

C	4.24062000	0.04364800	1.24893300
C	-0.10065000	-0.09823200	0.02484800
C	-6.55773600	-2.77109400	0.26318800
N	-8.82353700	-4.00947600	0.56766300
C	5.68596200	0.07360800	-1.19624000
C	4.28021100	-0.05460000	-1.18402000
C	-4.07266700	-1.49610300	-0.02236200
C	-0.44146900	-1.47320500	-0.12457900
C	-4.34557100	-2.69407600	-0.71162200
H	-3.56872400	-3.13203600	-1.33158100
C	6.31090200	0.41590700	-2.39776500
H	7.38628800	0.52340600	-2.40268900
C	5.64852200	0.19451900	1.27812800
C	-2.68012700	-0.94830300	-0.08869100
C	-2.32844600	0.46370500	-0.02787600
C	-5.07049800	-0.93519000	0.79490100
H	-4.87913000	-0.01729600	1.34290200
C	0.58742700	-2.44764800	-0.21946600
H	0.28850500	-3.48307700	-0.32303400
C	1.90540500	-2.05968000	-0.16348400
H	2.71191100	-2.78606500	-0.23361100
C	-6.30470600	-1.56863300	0.94383000
H	-7.06900600	-1.14358500	1.58925200

C	1.26713000	0.28353900	0.08994000
H	1.51851700	1.33701600	0.19137500
C	2.24957000	-0.68470400	0.00086200
C	4.20811600	0.43716600	-3.56428500
H	3.62878900	0.56989500	-4.47408900
C	5.59449100	0.59332700	-3.58458600
H	6.11762500	0.83298700	-4.50719500
C	-5.57743400	-3.32778700	-0.57869700
H	-5.78703400	-4.25078900	-1.11365100
C	-7.81902200	-3.44872600	0.43572300
C	-3.33023500	1.57299600	-0.08973300
C	6.45720100	-0.29774400	0.07165900
C	6.23525300	0.69950300	2.44320900
H	7.30830800	0.86601500	2.46792600
C	3.48361400	0.29139300	2.40796100
H	2.41059900	0.14223900	2.39918000
C	-4.31769600	1.60270500	-1.08746300
H	-4.37250600	0.78950800	-1.80328300
C	-3.24129200	2.63479700	0.82550800
H	-2.45183700	2.63128000	1.57225500
C	5.48079600	0.97951300	3.58756800
H	5.97034500	1.36149500	4.47947600
C	4.10536500	0.74915300	3.57149900

H	3.50271200	0.93194000	4.45912700
C	-5.20784800	2.67146200	-1.17732100
H	-5.95641300	2.70465700	-1.96510500
C	6.52255300	-1.85384000	0.12962900
H	7.04644900	-2.23576100	-0.75571600
H	7.06195000	-2.17144400	1.02769400
H	5.51786000	-2.29072300	0.15805900
C	7.90311900	0.23819900	0.06981200
H	7.93157600	1.33357700	0.00192400
H	8.42581500	-0.07261400	0.98177800
H	8.46674500	-0.18012200	-0.77230300
C	-4.15376600	3.68599600	0.77470000
H	-4.11525700	4.48164100	1.51222900
C	-5.13203200	3.71347500	-0.23541700
N	-6.78221900	5.71912500	-0.37616700
C	-6.05073400	4.82368700	-0.31210900

DMAC-CNQ (crystal)-S₁

N	-1.71316900	-1.87303500	-0.17018500
N	3.64066800	-0.25661600	0.02996100
N	-1.08720700	0.87955100	0.03559700
C	3.53474800	0.10742100	-2.36439200

H	2.45965600	0.00580000	-2.31334500
C	4.26442800	0.00088200	1.23364400
C	-0.10955000	-0.06046900	0.00236500
C	-6.56264900	-2.78173900	0.23512700
N	-8.82941600	-4.02300200	0.50974800
C	5.70877100	0.10376100	-1.19896600
C	4.29165600	-0.03082400	-1.17197400
C	-4.06413100	-1.49302300	-0.02612700
C	-0.43704300	-1.46149000	-0.12882100
C	-4.30889600	-2.73681700	-0.65080300
H	-3.49957400	-3.20071000	-1.20640800
C	6.31375000	0.38387600	-2.41919700
H	7.38830500	0.47035500	-2.45268500
C	5.68105800	0.19727400	1.27441800
C	-2.68900800	-0.93015100	-0.09491600
C	-2.35940700	0.44553500	-0.03644600
C	-5.10481000	-0.90874800	0.72807500
H	-4.93399000	0.03409900	1.24043100
C	0.62065000	-2.41471900	-0.19576700
H	0.34409800	-3.45807100	-0.28650300
C	1.95373200	-2.01664700	-0.12497400
H	2.75682300	-2.74937600	-0.17843100
C	-6.33897200	-1.54059800	0.85986700

H	-7.12832500	-1.08906900	1.45595300
C	1.24695900	0.32976400	0.06994300
H	1.48498500	1.38761900	0.15070100
C	2.24955500	-0.65679700	0.01088900
C	4.17433200	0.40966100	-3.55674700
H	3.59219400	0.54281600	-4.46257300
C	5.56905400	0.54693200	-3.59329300
H	6.07812800	0.77136900	-4.52747400
C	-5.53938400	-3.37268600	-0.53153400
H	-5.71897100	-4.32777900	-1.02008000
C	-7.82279000	-3.46026400	0.39194900
C	-3.36143100	1.55324100	-0.08614400
C	6.50589400	-0.21081700	0.05993800
C	6.24022500	0.64980600	2.46386100
H	7.30692300	0.84253200	2.51722500
C	3.48098800	0.15107900	2.41066500
H	2.41581800	-0.03149300	2.36679500
C	-4.35289400	1.60568200	-1.08085700
H	-4.40556500	0.80178100	-1.80643900
C	-3.26946000	2.61101500	0.83597000
H	-2.47294000	2.59571700	1.57484100
C	5.45268800	0.86908600	3.60546100
H	5.92118000	1.24586500	4.51056900

C	4.07834700	0.59438500	3.58094000
H	3.47205200	0.73535200	4.47180400
C	-5.24569200	2.67280600	-1.15157100
H	-5.99797900	2.71563900	-1.93564900
C	6.66712800	-1.77107000	0.11006100
H	7.20167000	-2.11278600	-0.78418500
H	7.24227600	-2.04829900	0.99888400
H	5.69376700	-2.27345900	0.15183800
C	7.91594400	0.41631700	0.05423000
H	7.87482300	1.51123400	-0.00453500
H	8.46499300	0.12870800	0.95762700
H	8.49775500	0.03982300	-0.79408900
C	-4.18052100	3.66324800	0.80460200
H	-4.13759500	4.45025000	1.55156300
C	-5.16738100	3.70471800	-0.19796600
N	-6.81323200	5.71503300	-0.31248000
C	-6.08322000	4.81680000	-0.25889300

DMAC-CNQ (crystal)-T₁

N	-1.70641500	-1.86581200	-0.28885900
N	3.61977200	-0.29780700	0.06072200
N	-1.08929900	0.85900500	0.17643600

C	3.51294100	0.06559200	-2.34845100
H	2.43301700	-0.00014800	-2.29199000
C	4.25055300	0.08707100	1.25304500
C	-0.11006300	-0.09413200	0.12301800
C	-6.54478400	-2.78320500	0.31486500
N	-8.80820800	-4.01942200	0.63249400
C	5.67859900	0.04271700	-1.20619500
C	4.27339800	-0.10045000	-1.17155200
C	-4.05394600	-1.49323300	0.00162300
C	-0.44996800	-1.46877300	-0.19840600
C	-4.30026600	-2.75486100	-0.59343300
H	-3.49975600	-3.22620400	-1.15435100
C	6.28044700	0.34588200	-2.42947800
H	7.35445600	0.45761100	-2.46212100
C	5.66062200	0.25473300	1.26387200
C	-2.69751200	-0.92194000	-0.10266000
C	-2.35533500	0.44969700	0.01807300
C	-5.09170800	-0.89400600	0.75480600
H	-4.92052200	0.05861300	1.24762800
C	0.61986800	-2.40416900	-0.43021400
H	0.33597200	-3.42577000	-0.64556200
C	1.95115800	-2.01489000	-0.35234000
H	2.75172800	-2.72446300	-0.54934300

C	-6.31985300	-1.52760000	0.91211500
H	-7.10570400	-1.06687300	1.50552700
C	1.22486100	0.25136300	0.32304700
H	1.47937800	1.28702500	0.53678100
C	2.27254500	-0.71771800	0.06169700
C	4.14509700	0.35523000	-3.55401900
H	3.55353000	0.49374100	-4.45390300
C	5.53584200	0.49808100	-3.60168400
H	6.03835100	0.72837500	-4.53831200
C	-5.52812700	-3.38936700	-0.44804800
H	-5.71049200	-4.35481600	-0.91437800
C	-7.80308600	-3.45904700	0.49537600
C	-3.34940600	1.56337000	-0.07194600
C	6.47303800	-0.24294000	0.06328900
C	6.24864300	0.73343000	2.43626900
H	7.32127600	0.89831000	2.46647900
C	3.49845800	0.26822000	2.43257400
H	2.43909900	0.04310900	2.43778200
C	-4.29851900	1.60013600	-1.10816400
H	-4.32358400	0.78698700	-1.82600400
C	-3.29352700	2.62960600	0.84147700
H	-2.52923400	2.62604800	1.61369300
C	5.49185400	0.99444200	3.58586000

H	5.98442600	1.36805600	4.47956900
C	4.11843400	0.74049900	3.58692400
H	3.52758500	0.89065300	4.48756900
C	-5.18587700	2.66730400	-1.23012800
H	-5.90464800	2.70026800	-2.04551200
C	6.59597800	-1.79644700	0.17662600
H	7.09961700	-2.19226500	-0.71418300
H	7.18444100	-2.05478500	1.06103300
H	5.61092000	-2.27008700	0.26302300
C	7.89783000	0.34747300	0.02305500
H	7.88383700	1.43980800	-0.08275100
H	8.44531100	0.08720500	0.93575500
H	8.46552200	-0.07991400	-0.81133800
C	-4.20314700	3.68130300	0.75752800
H	-4.19211400	4.47690100	1.49624700
C	-5.14551300	3.71064400	-0.28661200
N	-6.78369600	5.72015000	-0.49434100
C	-6.05744700	4.82261900	-0.39956000

DMAC-CNQ (amorphous)-S₀

N	1.63891200	-1.78971300	-0.42879600
N	-3.72677900	-0.15619600	-0.10146600

N	1.02314700	0.79564200	0.48022600
C	0.35141500	-1.37403400	-0.32619600
C	-1.33263600	0.30376700	0.32840600
N	8.99567200	-2.92622100	-1.61570000
C	2.58327000	-0.95026500	-0.07129700
C	4.00556700	-1.38777500	-0.28757300
C	0.03165500	-0.07962600	0.16873500
C	-2.34568600	-0.50013400	-0.17189900
C	-4.60689500	-1.06306100	0.55032100
C	4.69688200	-2.19655500	0.62975600
C	5.87477400	-1.53653000	-1.82111800
C	5.99601600	-2.63518000	0.35172500
C	6.58420300	-2.30174300	-0.88033300
C	-6.81692400	-1.69820100	1.30627000
C	-6.00361300	-0.84659700	0.54128500
C	-4.93228200	-3.00389000	2.00955700
C	-4.09880700	-2.16502700	1.27179600
C	-0.70235100	-2.21878100	-0.76890800
C	-4.20776100	1.12342300	-0.49610900
C	2.26651500	0.38756700	0.37414000
C	-6.30430200	-2.75854000	2.05270000
C	-5.60494300	1.36980800	-0.55492900
C	-1.99972800	-1.76820800	-0.75667400

C	4.61192400	-1.04439700	-1.50683100
C	-3.32862100	2.16112600	-0.87914900
C	3.38931800	1.33364600	0.66801800
C	-6.62834600	0.24961300	-0.32248800
C	-6.04471300	2.62330800	-1.00666900
C	7.92443900	-2.69747800	-1.23985200
C	-3.80181000	3.41802300	-1.25455000
C	4.33007100	0.99863600	1.65566800
C	3.57168500	2.49902700	-0.09389800
C	-5.17124300	3.65962000	-1.33428100
C	5.46824200	1.77595300	1.84492200
C	-6.98191900	-0.33720300	-1.71585100
C	4.71288000	3.28516900	0.08245400
C	-7.95010000	0.74493800	0.32097900
C	5.67545200	2.90577500	1.03389800
N	7.96000800	4.11963000	1.27609100
C	6.92176600	3.62005700	1.16239400
H	-1.53659600	1.24250600	0.83346300
H	4.21624200	-2.49026800	1.56176600
H	6.30268400	-1.38993400	-2.80545300
H	6.54120900	-3.24452600	1.06920600
H	-7.88771800	-1.52578500	1.31958700
H	-4.49363400	-3.82873000	2.56801100

H	-3.03691500	-2.36135800	1.27467900
H	-0.42799900	-3.20015600	-1.14022000
H	-6.96591900	-3.36943300	2.65971500
H	-2.79872700	-2.38928900	-1.15424700
H	4.06452400	-0.44877000	-2.23445100
H	-2.26160200	1.99614300	-0.91123600
H	-7.11237900	2.79580800	-1.10793500
H	-3.08645300	4.20079900	-1.49884700
H	4.17765700	0.11138200	2.26511200
H	2.84092800	2.76823300	-0.85365900
H	-5.55500500	4.62501800	-1.65612700
H	6.20566200	1.50773600	2.59748300
H	-6.08239400	-0.70273200	-2.22559700
H	-7.43560600	0.44864100	-2.33258700
H	-7.69825700	-1.16162000	-1.60262700
H	4.87378800	4.17048300	-0.52732700
H	-8.72431500	-0.02432500	0.22468700
H	-8.34001000	1.64109000	-0.16908600
H	-7.81626300	0.94969300	1.38671000

DMAC-CNQ (amorphous)-S₁

N	1.62725400	-1.75865600	-0.47203600
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N	-3.76331300	-0.15430000	-0.12089100
N	0.99333000	0.83581700	0.50339700
C	0.34239800	-1.32240800	-0.40181000
C	-1.35528900	0.30082800	0.34038800
N	8.96246000	-2.93100300	-1.62005900
C	2.57057100	-0.90707500	-0.04060400
C	3.98546800	-1.37052700	-0.25340500
C	0.02149800	-0.03615100	0.16102100
C	-2.34606700	-0.49245500	-0.26982100
C	-4.59685200	-1.05265600	0.54303900
C	4.64663900	-2.24798200	0.62331500
C	5.88090600	-1.47825500	-1.76335900
C	5.94056800	-2.70132100	0.34311200
C	6.55859300	-2.31198700	-0.85806200
C	-6.76344800	-1.63475000	1.45701200
C	-6.00057700	-0.80872200	0.63166700
C	-4.84511000	-3.00455300	1.99150900
C	-4.05146000	-2.19859500	1.18853300
C	-0.69581800	-2.12227700	-0.92778900
C	-4.24418000	1.06729700	-0.56942700
C	2.26980900	0.39505400	0.39997300
C	-6.20325900	-2.70422800	2.16228500
C	-5.65192700	1.35556400	-0.55129600

C	-2.02235800	-1.67432100	-0.94557700
C	4.62269800	-0.98103900	-1.44316000
C	-3.33734100	2.07128600	-1.02307200
C	3.39174200	1.33223100	0.69746200
C	-6.65585700	0.25153400	-0.23907200
C	-6.07391100	2.60800800	-0.99184200
C	7.89511900	-2.70931000	-1.22759100
C	-3.79601900	3.34146300	-1.34010500
C	4.35796200	0.97892300	1.65844400
C	3.57382800	2.51981900	-0.03670700
C	-5.16736700	3.61476800	-1.34900500
C	5.51084700	1.73696200	1.83277400
C	-6.99608000	-0.41421500	-1.61157800
C	4.72500500	3.29105400	0.12629000
C	-7.98527100	0.74812400	0.37879200
C	5.71153000	2.88431200	1.04506900
N	8.00926400	4.07653800	1.26178100
C	6.96547900	3.58409300	1.15955000
H	-1.59648100	1.19500600	0.90806700
H	4.14455900	-2.57579700	1.53240400
H	6.33299800	-1.28142100	-2.72721100
H	6.46046500	-3.36012600	1.03554100
H	-7.82237400	-1.43671700	1.55943500

H	-4.39774800	-3.85516200	2.49999600
H	-3.00435200	-2.42849300	1.06055700
H	-0.40406500	-3.07834900	-1.34453000
H	-6.82741100	-3.29406300	2.82880500
H	-2.80028100	-2.27424800	-1.41211400
H	4.09971900	-0.33042000	-2.14054000
H	-2.28190200	1.85476600	-1.10030700
H	-7.13562300	2.82801500	-1.03889700
H	-3.08219900	4.11873000	-1.59727400
H	4.20667000	0.08437300	2.25646000
H	2.83446800	2.80476100	-0.78200100
H	-5.53377300	4.59541600	-1.64335000
H	6.26402700	1.44364900	2.56036400
H	-6.08236200	-0.75229400	-2.11351600
H	-7.49850200	0.31986500	-2.25229900
H	-7.66260500	-1.27061900	-1.44957900
H	4.88268300	4.18411900	-0.47376000
H	-8.73719800	-0.04673700	0.32898400
H	-8.39775400	1.59866800	-0.16998700
H	-7.85874100	1.02734700	1.42769400

DMAC-CNQ (amorphous)-T₁

N	1.62652500	-1.80318300	-0.37823600
N	-3.73719300	-0.18705200	-0.10391200
N	1.01660200	0.84808700	0.43665400
C	0.36718900	-1.37502100	-0.31702400
C	-1.31734900	0.32337300	0.26769800
N	8.96018800	-2.99281000	-1.62612400
C	2.59546600	-0.90892300	-0.02199200
C	4.00247500	-1.37926600	-0.25079900
C	0.04158600	-0.03837500	0.12991800
C	-2.38350900	-0.55298000	-0.23341200
C	-4.64557600	-1.08549500	0.52473300
C	4.68558700	-2.21219800	0.65295400
C	5.85701800	-1.56902200	-1.80320300
C	5.97348700	-2.67568500	0.36472600
C	6.56045300	-2.34887900	-0.87023400
C	-6.86538300	-1.67094800	1.28427800
C	-6.03867800	-0.83685900	0.51484100
C	-4.99056100	-2.98821600	2.02082600
C	-4.14670800	-2.18084400	1.26837600
C	-0.70455000	-2.24116000	-0.72133200
C	-4.19732600	1.08813300	-0.51377700
C	2.29299200	0.39868400	0.36555100
C	-6.36234600	-2.72238200	2.04820700

C	-5.58973100	1.38157400	-0.54096600
C	-2.03219400	-1.82124600	-0.71764700
C	4.60711900	-1.05290300	-1.47643900
C	-3.28131600	2.07467200	-0.95492700
C	3.40535300	1.34994500	0.66590600
C	-6.64085800	0.28953500	-0.31894800
C	-5.98710500	2.65337600	-0.97323700
C	7.89360600	-2.75752900	-1.24012400
C	-3.70986700	3.36413100	-1.25818600
C	4.35796000	1.01354200	1.64355700
C	3.57884900	2.53076700	-0.07775300
C	-5.07198500	3.66078000	-1.28346600
C	5.50060300	1.78592800	1.82509600
C	-7.01545800	-0.26005300	-1.72653800
C	4.72169200	3.31464800	0.09154100
C	-7.94598700	0.80794200	0.33993000
C	5.70003100	2.92402700	1.02413300
N	7.99564500	4.11873100	1.25097700
C	6.95122900	3.62988300	1.14271400
H	-1.55420700	1.23338900	0.81083400
H	4.20672200	-2.49648000	1.58879000
H	6.28190100	-1.42666300	-2.78959800
H	6.51297800	-3.29557100	1.07770700

H	-7.93325700	-1.48391500	1.29945400
H	-4.56712700	-3.80402200	2.60262300
H	-3.08513800	-2.37963300	1.27024700
H	-0.41874100	-3.22231400	-1.08320100
H	-7.03191400	-3.30987200	2.66913300
H	-2.80862200	-2.48364300	-1.09365200
H	4.06598200	-0.44121300	-2.19501200
H	-2.23293000	1.83839100	-1.07963800
H	-7.04665100	2.87071400	-1.06683300
H	-2.97626300	4.12252000	-1.52008700
H	4.20813000	0.12335200	2.24869400
H	2.83921300	2.80649500	-0.82646100
H	-5.42099900	4.64786800	-1.57791800
H	6.24740200	1.50861100	2.56526200
H	-6.12933300	-0.63738400	-2.25040300
H	-7.45478700	0.54876100	-2.32340100
H	-7.75133600	-1.06787100	-1.62443300
H	4.87574600	4.20587600	-0.51193400
H	-8.74464000	0.06730700	0.22426500
H	-8.30746300	1.72663400	-0.12945600
H	-7.80430300	0.98452200	1.40962800

References

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