Electronic Supplementary Information
for

Alignment of Paired Molecules of C_{60} within a Hexagonal Platform Networked through Hydrogen-Bonds

Ichiro Hisaki,[a]* Shoichi Nakagawa,[a] Hiroyasu Sato,[b] and Norimitsu Tohnai[a]

[a] Department of Material and Life Science, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan.

[b] Rigaku Corporation, Matsubara-cho 3-9-12, Akishima, Tokyo 196-8666, Japan.

1. General

Single crystal X-ray measurement and analysis. For crystals **T18-C_{60}-1** and **T18-C_{60}-2**, diffraction data were collected on a two-dimensional X-ray detector (PILATUS 200K/R) equipped in Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Cu-Kα radiation (λ = 1.54187 Å). For crystal **T18-*o*DCB**, diffraction data were collected on a CCD (MX225HE, Rayonix) with the synchrotron radiation (λ = 0.8000 Å) monochromated by the fixed exit Si (111) double crystal. The cell refinements were performed with a software CrysAlisPro 1.171.38.41o. SHELXT were used for the structure solution of the crystals. All calculations were performed with the observed reflections [I > 2σ(I)] with the program CrystalStructure crystallographic software packages, except for refinement which was performed by SHELXL. All non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were placed in idealized positions and refined as rigid atoms with the relative isotropic displacement parameters. SQUEEZE function equipped in the PLATON program was used to remove disordered solvent molecules in the cavities for **T18-*o*DCB**. Synchrotron radiation experiments were undertaken at BL38B1 in SPring-8 with approval of JASRI.

2. SCD searches on C_{60} contained crystal structures.

Table S1. Classification of C_{60} crystals extracted from the CSD.

assembly	Refcodes
Discrete monomer	CISWEI, ABOSUF, ABOSUF01, ALOTAX, BEKGOO, BODCEE, BODCUU, BODDEF, BOXQOU, CAJFOJ, CELTIW, CELVAQ, CEMPAL, COVBAR, DIBHIH, DIBHON, DIZVEP, DIZZIW, EHICOO, ELUNEE, EWIMUT, FERYEI, FEXLUQ, FEXMAX, FOPYEO, FOPYEO01, GALGIL, GALGIL01, GAMSUK, GAMTAR, HOBXUT, HOBYAA, HOBYEE, HOBYII, HOBYOO, IPIZAJ, IXIKIJ, IYODUW, JAXYIQ, JAYDIW, KEQKIA, LAZPAD, LAZPAD01, LISZET, LIZSET, LOHSOQ, MEQGIY, MIWYOH, MOSFIJ, MOSFOP, OCOJIB, OCOLOJ, OLUKAH, PEHGEP, PUJROB, QARQIJ, QEBKIT, RAWXAQ, RAZGIJ, SAMCIU, SEGWUX, TADQAQ, TIKHAW, TORJIU, TUDCOK, TUQTAA, UDUZUQ, UFABAG, UFOMAD, ULEHAU, UPEKOQ, UTUBAN, UTUBER, VAVVIY, VAZXAW, VEMPEI, VUPBAK, XAGBUE, XAGCAL, XAGCEP, XAGCIT, XEQHAD, XEQHEH, XEYZAC, XIHZOE, XOBDAU, XOBDEY, XOFCOK, XOFFAA, XONVOM, YALFOH, YAPXET, YECJEW, YECJOG, YEMTUH, YIKVET, YOFLEM, YOLSOH, YUXCAV01, YUXCEZ, YUXCEZ01
Discrete dimer	BIBVUE, DAYXAE, FUMBIZ, LIZSIX, NIFXUV, NIFYAC, VAJYIP, DIBHUT*, FEXMEB* (*: C_{60} anions are included)
one-dimensional array	SOBLOM, EWINAA, FAJFAX, HIVKEC, HULLIJ, LIPKEB, LUDCET, MABPEL, MOCFIU, MUDJEB, NIDNUK, QADQIW, RIBCEL, SEGWOR, UBOJIE, UDUYID, UTAYOE, WIJMOS, ZAPNEJ, HONKAY, DIDREP, FOPZEP, FOPZEP01, KUMMEK, MESHOI, MOSGAC, MUJLUZ, NAGNAK, NIDPAS, PASQIL, QARQEF, QOWCUB, QOWDAI, RAXYEW, SUGBUR, VAGKEV, VAVVUK, VEMNOQ, VEMQAF, WOCJIJ

Table S1. Continued.

two-dimensional array	VOPNEV, VOPNIZ, ALOTIF, BAQRUG, BODDIJ, CEGCIB, CEMNUD, DIBHED, GAQLUG, HOSJAA, HULLAB, HULLEF, HULLOP, IFOMAT, IXUXAB, IXUXAB04, JOHTOR, KUVNOE, LITPUZ, NAJJEP, NAJJIT, NAPPOJ, NIGPOI, NIXPOZ, OFAYOL, OKOQIO, PASQAB, PATVIQ, PIQHOM, QARPUU, QARPUU02, QARQAB, QAVJON, QIYSUN, QIYTAU, QIYTEY, QIYTIC, QIYTOI, QIYVAW, QIYVEA, SADWAV, UBOJOK, UFUQER, UKAGIW, UVONAV, VEPTIV, VEQSIV, XAYXOK, XISQAS, XOCJII, YEHLAZ, YEHLED, YEKBOF01, YICLUT, ZESHIO
Three-dimensionally spreaded arrangement	MIPSEL, ABOSOZ, ADACIR, AJEJAA, ATEMER01, BAQLOW, BAQLOW01, BIMGIP, CEBCES, CELYOH, CIMZAA, COGYEE, COGYEE01, COXLUX, COXMAE, COXMEI, COXMIM, COXMOS, COXMUY, COXNAF, COXNEJ, FIBVIV, FULLER, GEXQUV, GIPWUY, HASHIU, HEGPAK, HEGPAK01, HIBPUF, IBIDIH, IBIGUW, IBIHAD, INEMUJ, JEVBAO, JOCSOJ, JUGCET, JUVYAA, KEVMUV, KEVNAC, KEVNEG, KIWFEC, KUGGIC02, LAVNIF, LEKFEN, LUGKUT, LUGLEE, MIMROP, MOBWUX01, MOSGEG, MULFOO, MULFOO01, MUPZUS, MUVHIV, NIRLOP, NIYBOM, NOBLEV, NUDDIZ, NUDDIZ02, NUHJUV, NUSVAY, OSEYER, PABKEJ01, POSHOU, POSHOU01, PUHJOR, PUHJIL, PUKHAE, QEJPAX, QEJPAX01, QEJPAX02, QIYTUO, QUFLUY, RAXYAS, SADVUO, SASMAB, SEPDIB, SEPDOH, SOCTOT, SOMGIK, SOMGIK01, TAWKEH, TEYCEF, TONDUV, UBOJUQ, UFUQAN, UJAFAM, UJAFEQ, UJAFIU, UJAFOA, UKAREE, ULEHEY, UPOYII, VAVVOE, XEJDAT, XEJDEX, XEXBUY, XONWAZ, YEHKIG, YEHKUS, YEHLIH, YOFQOA, YUGWUT