Electronic Supplementary Material (ESI) for CrystEngComm.

Two–component organic crystals without hydrogen bonding: structure and intermolecular interaction in bimolecular stacking

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Electronic Supplementary Information

Table ESI S1.122 refcodes NOHB-ALL dataset;space group,density,T/K,year,R

ADULEQ03	'C 2/m'	1.404	297.0	2002.	4.80
FOMQUU	'P -1'	1.544	174.0	2005.	4.30
GOHYUZ	'P 21/m'	1.511	297.0	2012.	6.05
MOCCEM	'C 2/c'	1.450	173.0	2002.	4.30
NOKDAS	'P 21/n'	1.409	185.0	1997.	4.50
WAWPAM	'P 21/n'	1.598	174.0	2005.	3.20
ACNTCQ	'P -1'	1.278	295.0	1973.	6.30
ANTCYB14	'P 21/a'	0.000	138.0	1980.	4.50
BORPAA	'P 21/n'	1.395	173.0	2009.	4.23
BORPII	'P 21/n'	1.409	173.0	2009.	5.56
BUHSIG	'C -1'	0.000	295.0	1983.	6.30
BZQTCQ10	'P 21'	1.277	295.0	1980.	4.40
CHRTCQ01	'P -1'	1.388	100.0	2014.	3.30
CIFWUJ	'C 2/m'	0.000	295.0	1984.	4.40
DURYUK	'P 21/a'	1.311	295.0	1986.	3.40
GIGCEE	'P -1'	1.368	295.0	1988.	3.50
HIGPUJ	'P -1'	1.323	100.0	2007.	6.52
JOCVEC01	'P -1'	1.326	295.0	1999.	3.90
KARHAM	'P 21/a'	1.210	295.0	1989.	3.80
LIYSIV	'P -1'	1.331	100.0	2000.	4.27
LOCVOO01	'P 21/c'	1.330	295.0	1999.	7.30
PYRCBZ02	'P 21/c'	1.357	173.0	2012.	6.30
PYRTCQ02	'P 21/n'	1.344	100.0	2014.	3.37
REHMUM	'P 21/c'	1.352	295.0	1996.	3.32
RUXMON	'P -1'	1.217	173.0	2010.	7.42
TCQBDX	'P 21/c'	1.361	295.0	1973.	4.30
TCQMHP	'C m'	1.336	295.0	1973.	4.90
TCQNAP01	'P -1'	1.345	100.0	2014.	2.92
TCQPEN10	'P -1'	1.344	295.0	1973.	7.10
TPDTCB01	'P -1'	1.256	298.0	2004.	4.09
VERJUY01	'P 21/c'	1.286	100.0	2006.	3.27
JOCRIC01	'P 21/n'	1.522	295.0	1999.	5.70
ASAKIO	'P 21/n'	1.671	120.0	2004.	3.99
ASAKOU	'P -1'	1.718	120.0	2004.	4.88
ASIJER	'P -1'	1.569	160.0	2004.	6.75
BICVUE01	'P 21/a'	0.000	165.0	1992.	3.30
ECUTUR	'P 21/n'	1.648	120.0	2001.	4.01
ECUVIH	'P -1'	1.652	120.0	2001.	4.42
ECUVON	'P -1'	1.637	120.0	2001.	4.20
IVOBOK	'C 2/c'	1.565	180.0	2002.	4.96
JOCRIC	'P 21/n'	1.574	165.0	1999.	5.30
NPOFNP	'P 21/c'	1.671	295.0	1975.	6.50
OCAYIA01	'P 21/n'	1.556	223.0	2001.	3.21
TIJTUB01	'P 21/c'	1.514	90.0	2001.	6.64
XUNJAR	'P 21'	1.696	120.0	2002.	6.20
ZZZGKE01	'P 21/c'	1.563	200.0	2002.	4.41
ZZZGMW02	'C 2/c'	1.576	150.0	2002.	5.01
DMAFBZ01	'P -1'	1.566	120.0	1985.	6.00
FOJGOC	'P -1'	1.406	173.0	2014.	4.61
FOJGUI	'P -1'	1.441	100.0	2014.	3.10
FOJSAY	'P -1'	1.623	295.0	1987.	4.00
KARCIQ01	'P -1'	1.661	173.0	2005.	4.02
LAPSAX	'P 1'	1.607	293.0	2005.	5.21
LAPSEB	'C 2/c'	1.589	293.0	2005.	4.72
ELIQIZ	'R -3 m'	1.010	123.0	2003.	4.07
GURNIR	'P n m a'	0.982	168.0	2010.	6.14
KURCEG	'P 21/c'	1.157	173.0	2010.	3.58
APANBZ	'P -1'	0.000	123.0	1966.	4.70
ASKNBZ	'P 21'	0.000	295.0	1978.	5.20
CECPEF	'P -1'	1.324	295.0	1999.	6.10

DBTTNB	'P -1'	1.510	295.0	1977.	3.00
GEXMED	'P 21/c'	1.806	293.0	2013.	4.56
NIBJUF	'P 21/c'	1.640	293.0	2013.	5.42
PVVBFD01	'P 21'	1.461	293.0	2003.	6.13
RUYKUR	'P 21/n'	1.514	120.0	2003.	5.98
RUYLAY	'P 21/n'	1.545	120.0	2003.	4.90
URIJEL	'P 21/c'	1.515	95.0	2010.	4.55
URIKEM	'P -1'	1.677	95.0	2010.	3.72
URIKUC	'P -1'	1.496	95.0	2010.	5.92
URILEN	'P 21/n'	1.501	95.0	2010.	6.47
VIGKIF	'P n a 21'	1.442	295.0	1991.	3.90
XAHZAH	'P 21/c'	1.399	295.0	2000.	5.99
ANTPML01	'P -1'	0.000	153.0	1978.	4.60
BECNUS10	'P -1'	0.000	295.0	1982.	6.30
DURZAR01	'P 21/a'	1.552	120.0	1986.	3.70
FILHIR	'P 1 1 21/n'	1.450	295.0	1987.	4.10
FILHOX	'P -1'	1.490	295.0	1987.	2.90
NAPYMA01	'C 2/m'	1.460	295.0	1979.	5.30
PYRPMA02	'P 21/a'	1.480	295.0	1989.	4.90
BAZDAH	'P 21/c'	0.000	295.0	1981.	3.40
BZPCBQ	'P 21/c'	1.471	295.0	1977.	6.50
CAFWAH	'P -1'	1.645	295.0	1983.	4.60
CHRFAN	'P 21/c'	1.561	295.0	1975.	7.00
CLAHMB02	'P 21/n'	1.526	423.0	2000.	3.68
CORPIJ	'P 43'	1.486	130.0	2009.	5.48
FUDTUT	'P -1'	1.792	295.0	1987.	4.80
MOTRES	'P b c n'	1.539	296.0	2002.	5.40
PYRFLR01	'P 21/n'	1.592	200.0	1996.	3.80
CAPTOC01	'P 21/c'	0.000	295.0	1984.	3.48
CEKBUP	'P 21/a'	1.430	295.0	1984.	4.90
CEWYOT	'P 21 21 21'	1.468	293.0	2006.	4.47
DNPCPH	'P -1'	0.000	120.0	1975.	4.80
FOZHAD	'P 21'	1.660	120.0	1987.	3.20
GIFMUD	'P n a m'	0.000	295.0	1988.	5.50
HAFVEQ	'P 21/a'	1.338	200.0	2003.	4.06
IDENEM	'C m'	1.705	291.0	2013.	4.98
KIZVAQ	'P 21 21 21'	1.382	295.0	2000.	6.30
KOBFIQ	'P 21/a'	1.368	295.0	2000.	6.40
MXTTCQ01	'P 21/c'	1.400	295.0	1982.	5.00
NEMHIW	'P 21'	1.690	173.0	2001.	3.26
NHAZMS02	'P -1'	1.640	295.0	1984.	3.98
NUCQEH	'P -1'	1.439	173.0	1997.	3.95
NUWGUH	'P n a 21'	1.371	173.0	1997.	5.88
PANCYQ	'P c a 21'	1.485	295.0	1978.	5.60
PYRBZQ01	'P 43'	1.414	100.0	2009.	4.50
QILZOA	'P 21/n'	1.481	295.0	2001.	4.00
QOTCEH	'P 21/n'	1.526	123.0	2001.	4.46
RAYLOS	'P -1'	1.276	295.0	1996.	5.40
REDCIM	'P 21/n'	0.000	200.0	1996.	3.32
REDDAF	'C 2/c'	1.346	220.0	1996.	4.42
REYPIU	'P -1'	1.542	295.0	1996.	5.50
RUXMAZ	'P -1'	1.241	173.0	2010.	4.49
RUXMED	'P -1'	1.184	173.0	2010.	4.43
RUXMIH	'P -1'	1.220	173.0	2010.	3.53
RUXMUT	'P -1'	1.175	200.0	2010.	4.56
RUXNAA	'P n m a'	1.219	173.0	2010.	4.34
SAKLAR	'P -1'	1.456	295.0	1988.	3.80
SENYIV	'P n a 21'	1.614	173.0	2012.	4.85
VIHGOI	'P 21/n'	1.330	295.0	1990.	4.70
WABWEB	'P 21/a'	1.508	295.0	1993.	5.00
YUWNEJ	'P 21/c'	0.000	295.0	1995.	4.46
ZEZHAP	'P n m a'	1.765	95.0	2012.	3.56

Table ESI S2. CSD Refcodes of cocrystals in the NOHB-ENE dataset

ASAKIO	octafluoronaphthalene biphenyl
ECUTUR	octafluoronaphthalene anthracene
ECUVIH	octafluoronaphthalene pyrene
ECUVON	octafluoronaphthalene triphenylene
NPOFNP	octafluoronaphthalene naphthalene
XUNJAR	octafluoronaphthalene acenaphthene
OCAYIA01	octafluoronaphthalene diphenylacetylene
BICVUE01	hexafluorobenzene benzene
IVOBOK	hexafluorobenzene naphthalene
ZZZGMW02	hexafluorobenzene anthracene
ZZZGKE01	hexafluorobenzene pyrene
JOCRIC01	hexafluorobenzene dibenzocyclododecadiene-tetrayne
ANTPML01	pyromellitic anhydride anthracene
FILHIR	pyromellitic anhydride chrysene
FILHOX	pyromellitic anhydride tetracene
NAPYMA01	pyromellitic anhydride naphthalene
PYRPMA02	pyromellitic anhydride pyrene
BECNUS10	pyromellitic anhydride phenazine
ANTCYB14	1,2,4,5-tetracyanobenzene anthracene
BUHSIG	1,2,4,5-tetracyanobenzene biphenyl
PYRCBZ02	1,2,4,5-tetracyanobenzene pyrene
REHMUM	1,2,4,5-tetracyanobenzene perylene
VERJUY01	1,2,4,5-tetracyanobenzene tetramethylpyrazine
KARHAM	1,2,4,5-tetracyanobenzene durene
CIFWUJ	1,2,4,5-tetracyanobenzene diphenylacetylene
BORPII	2,3,5,6-pyrazinetetracarbonitrile pyrene
JOCVEC01	tetracyanoquinodimethane dibenzocyclododecadiene-tetrayne
ACNTCQ	tetracyanoquinodimethane acenaphthene
TCQPEN10	tetracyanoquinodimethane phenazine
TCQNAP01	tetracyanoquinodimethane naphthalene
CHRTCQ01	tetracyanoquinodimethane chrysene
HIGPUJ	tetracyanoquinodimethane tetracene
PYRTCQ02	tetracyanoquinodimethane pyrene
MOTRES	tetrafluoro-1,4-benzoquinone (fluoranil) triphenylene
PYRFLR01	tetrafluoro-1,4-benzoquinone (fluoranil) pyrene
CHRFAN	tetrafluoro-1,4-benzoquinone (fluoranil) chrysene
CAFWAH	tetrachloro-1,4-benzoquinone (chloranil) perylene
CORPIJ	chloro-1,4-benzoquinone pyrene
PYRBZQ01	1,4-benzoquinone pyrene
CEKBUP	naphthalene-1,4,5,8-tetrone pyrene
DNPCPH	tetrachlorophthalic anhydride naphthalene
FOZHAD	tetrachlorophthalic anhydride phenanthrene
FOMQUU	tetrachloro-1,4-dicyanobenzene anthracene
WAWPAM	tetrachloro-1,4-dicyanobenzene pyrene
PANCYQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone phenanthrene
RUXMON	1,4-dicyanobenzene 1,4-diethynylbenzene
GOHYUZ	tetrachloro-1,2-dicyanobenzene anthracene
PVVBFD01	1,3,5-trinitrobenzene triphenylene
VIGKIF	1,3,5-trinitrobenzene chrysene
CECPEF	1,4-dinitrobenzene 1,4-diethynylbenzene
REDCIM	3,5-dinitro-cyanobenzene pyrene
RUXMAZ	2,2'-bipyridyl 1,4-diethynylbenzene
KURCEG	benzene diphenylacetylene

Table ESI S2 (continued) Refcodes and energies in the NOHB-ENE dataset

cocrystal	coformers	PE_{tot}	PE_{exc}	E_{coul}	ΔU_{Coul}	E_{disp}	ΔU_{disp}
ASAKIO	OFNRES07*BIPHEN04	-205.2	-27.9	-70.6	-24.7	-227.3	-26.9
ECUTUR	OFNRES07 ANTCEN13	-218.4	-17.4	-77.9	-25.2	-252.8	-17.1
ECUVIH	OFNRES07 PYRENE02	-225.2	-22.9	-76.4	-28.8	-268.1	-31.8
ECUVON	OFNRES07 TRIPHE11	-217.8	-14.1	-74.5	-21.3	-262.3	-10.5
NPOFNP	OFNRES07 NAPHTA10	-190.4	-20.7	-60.0	-15.7	-197.9	-1.8
XUNJAR	OFNRES07 ACENAP03	-176.4	3.2	-67.3	-19.0	-212.8	-4.2
OCAYIA01	OFNRES07 DPHACT10	-181.6	6.1	-61.6	-11.1	-196.0	26.1
BICVUE01	HFBRES02*BENZEN18	-129.2	-18.6	-50.4	-15.1	-143.3	-16.0
IVOBOK	HFBRES02 NAPHTA10	-146.6	-6.9	-47.6	-3.9	-159.6	9.0
ZZZGMW02	HFBRES02 ANTCEN13	-176.6	-5.6	-56.6	-4.5	-208.4	-0.2
ZZZGKE01	HFBRES02 PYRENE02	-189.8	-17.5	-55.3	-8.3	-213.4	-4.6
JOCRIC01	HFBRES02 JOCQUN01	-171.2	7.3	-47.1	2.4	-190.0	36.4
ANTPML01	PYMDAN ANTCEN13	-219.6	4.2	-102.6	5.5	-253.9	-30.6
FILHIR	PYMDAN CRYSEN	-233.2	2.1	-109.8	3.7	-240.6	0.2
FILHOX	PYMDAN TETCEN01	-239.4	23.7	-83.1	36.6	-272.8	3.7
NAPYMA01	PYMDAN NAPHTA10	-186.8	5.7	-98.4	1.3	-180.8	2.9
PYRPMA02	PYMDAN PYRENE02	-224.0	1.1	-102.5	0.5	-236.4	-12.5
BECNUS10	PYMDAN PHENAZ04	-211.4	1.7	-93.3	14.1	-219.5	-19.4
ANTCYB14	TCYNBZ01 ANTCEN13	-221.8	3.6	-117.1	-19.4	-239.2	-14.8
BUHSIG	TCYNBZ01 BIPHEN04	-203.0	-1.3	-91.9	-1.0	-187.1	2.0
PYRCBZ02	TCYNBZ01 PYRENE02	-229.8	-3.1	-105.9	-13.3	-248.5	-23.5
REHMUM	TCYNBZ01 PERLEN04	-246.8	-1.4	-102.2	-4.1	-250.1	6.1
CIFWUJ	TCYNBZ01 DPHACT10	-203.4	8.7	-92.6	2.9	-203.0	7.9
KARHAM	TCYNBZ01 DURENE05	-188.8	-3.1	-99.9	-14.4	-185.2	-9.2
VERJUY01	TCYNBZ01 MPYRAZ01	-203.2	-8.3	-114.8	-16.7	-197.6	-15.1
TCQNAP01	TCYQME03 NAPHTA10	-203.4	4.1	-93.8	7.7	-233.2	-18.5
CHRTCQ01	TCYQME03 CRYSEN	-261.8	-11.5	-118.6	-3.3	-326.4	-54.6
HIGPUJ	TCYQME03 TETCEN01	-255.0	23.1	-108.1	13.4	-291.9	15.6
PYRTCQ02	TCYQME03 PYRENE02	-237.4	2.7	-107.0	-2.2	-277.9	-23.0
JOCVEC01	TCYQME03 JOCQUN01	-228.8	17.5	-73.2	34.1	-259.9	12.6
ACNTCQ	TCYQME03 ACENAP03	-193.0	24.4	-81.7	23.8	-222.8	4.4
TCQPEN10	TCYQME03 PHENAZ04	-217.4	10.7	-92.7	16.5	-224.9	6.2
MOTRES	TFBENQ TRIPHE11	-216.4	-31.9	-71.0	-2.4	-231.3	-20.4
PYRFLR01	TFBENQ PYRENE02	-211.6	-28.5	-86.1	-23.1	-230.7	-35.3
CHRFAN	TFBENQ CRYSEN	-230.8	-37.5	-86.3	-12.8	-244.6	-32.3
CAFWAH	TCBENQ07 PERLEN04	-252.8	-7.8	-82.0	9.6	-334.0	-28.6
CORPIJ	CLBENQ PYRENE02	-210.2	-15.6	-76.4	-8.2	-257.9	-40.2
PYRBZQ01	BNZQUI03 PYRENE02	-189.4	-8.5	-74.2	-3.2	-240.8	-41.6
FOMQUU	BAWNOC ANTCEN13	-227.0	5.5	-85.6	-2.3	-285.4	-9.9
GOHYUZ	BAWMUH ANTCEN13	-217.0	6.7	-69.8	13.6	-263.7	7.3
WAWPAM	BAWNOC PYRENE02	-253.6	-19.8	-84.9	-6.7	-311.8	-35.7
PANCYQ	CLCYBQ PHENAN08	-227.4	-19.6	-92.2	-12.8	-245.4	-18.7
CEKBUP	PYRENE02 BODCOM	-223.0	-0.6	-103.4	-9.0	-244.2	-11.2
DNPCPH	TECLPH20 NAPHTA10	-206.4	-4.1	-89.3	-14.0	-268.1	-28.7
FOZHAD	TECLPH20 PHENAN08	-245.8	-20.8	-99.4	-21.2	-305.3	-39.5
PVVBFD01	TNBENZ10 TRIPHE11	-212.0	-8.5	-86.4	-9.9	-234.5	3.7
VIGKIF	TNBENZ10 CRYSEN	-223.2	-10.9	-80.8	0.6	-245.6	-6.0
REDCIM	DINFOV01 PYRENE02	-220.6	-8.1	-84.0	2.1	-251.6	-27.3
RUXMAZ	ETYNBZ01 BIPYRL04	-196.8	-24.9	-101.6	-37.0	-200.7	11.7
RUXMON	ETYNBZ01 TEPNIT11	-162.6	-4.2	-75.1	-1.0	-158.3	9.9
CECPEF	ETYNBZ01 DNITBZ11	-161.2	11.3	-64.5	10.3	-151.0	26.5
BORPII	BORPUU PYRENE02	-233.8	-10.5	-96.5	6.1	-253.0	-32.6
KURCEG	BENZEN18 DPHACT10	-154.0	-9.1	-48.9	-7.7	-193.5	-9.8

*OFNRES and HFBRES are pseudo-refcodes for the crystal structures of octafluoronaphthalene and hexafluorobenzene obtained by molecular simulation.

Table ESI S2 (continued) Refcodes of coformers in the NOHB-ENE dataset

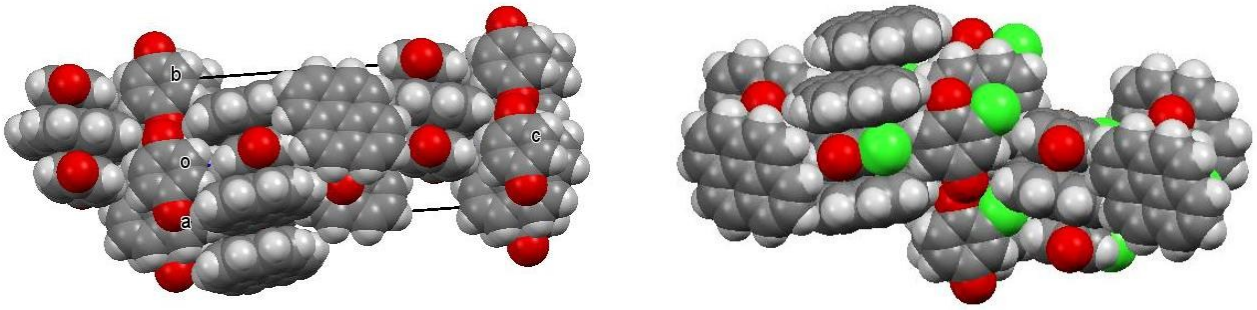
BIPHNE10	'P 21/a'	1.242	295.0	1966.	6.20
ACENAP03	'P c m 21'	1.221	295.0	1986.	3.80
ANTCEN13	'P 21/a'	0.000	259.0	1990.	3.50
BENZEN18	'P b c a'	1.050	150.0	2010.	5.54
BIPHEN04	'P 21/a'	0.000	295.0	1977.	6.30
BIPYRL04	'P 21/n'	1.326	123.0	2002.	2.98
BNZQUI03	'P 21/c'	1.366	173.0	2002.	4.29
BODCOM	'P 21/n'	1.592	295.0	1982.	6.50
BORPII	'P 21/n'	1.409	173.0	2009.	5.56
BORPUU	'P b c a'	1.410	173.0	2009.	4.81
CECPEF	'P -1'	1.324	295.0	1999.	6.10
CLBENQ	'P 21 21 21'	1.573	295.0	1970.	3.10
CRYSEN	'I 2/c'	0.000	295.0	1960.	8.00
DNITBZ11	'P 21/n'	1.618	295.0	1980.	4.08
DPHACT10	'P 21/c'	1.160	173.0	2011.	3.44
DURENE05	'P 1 1 21/b'	1.040	295.0	1977.	6.70
ETYNBZ01	'P 21/c'	1.202	125.0	1997.	5.38
JOCQUN01	'P 21 21 21'	1.311	295.0	1999.	4.50
JOCRIC01	'P 21/n'	1.522	295.0	1999.	5.70
MPYRAZ01	'P b c a'	1.150	295.0	1981.	8.40
NAPHTA10	'P 21/a'	0.000	239.0	1982.	3.50
OCAYIA01	'P 21/n'	1.556	223.0	2001.	3.21
PERLEN04	'P 21/c'	1.353	295.0	1998.	4.22
PHENAZ04	'P 21/n'	1.333	295.0	1991.	5.32
PYMDAN	'P 42/n'	1.680	295.0	1979.	3.80
PYRENE02	'P 21/a'	0.000	295.0	1972.	3.20
TCBENQ07	'P 21/c'	2.001	100.0	2007.	1.37
TCQPEN10	'P -1'	1.344	295.0	1973.	7.10
TCYNBZ01	'P 21/a'	1.372	295.0	1989.	3.90
TCYQME03	'C 2/c'	1.354	180.0	2015.	3.33
TECLPH20	'P 21/n'	1.980	295.0	1982.	3.30
TEPNIT11	'P -1'	1.285	295.0	1984.	4.26
TETCEN01	'P -1'	1.320	175.0	1999.	5.70
TFBENQ	'P 21/c'	1.915	295.0	1974.	6.60
TRIPHE11	'P 21 21 21'	1.308	295.0	1973.	4.80
VERJUY01	'P 21/c'	1.286	100.0	2006.	3.27

Table ESI 3. Computer-generated crystal structures for perfluorobenzene (pseudo-refcode HFBRES02) and perfluoronaphthalene (pseudo-refcode OFNRES07). Energies: AA, atom-atom CLP, or PIXEL

refcode	a	b	c	beta	density	lattice energy
HFBENZ02 P21/n Z'=3/2	5.904	9.117	16.775	94.01	2.058	-61.0 AA
HFBRES02 P21/c Z'=1/2 from polymorph generator	5.30	5.71	9.96	95.2	2.057	-65 AA -52.0 PIX** DHsubl 49.0
OFNRES07 one component from OFNAPH07						-83.2 AA -79.4 PIX** DHsubl 79.4

With MP"/6-31G electron density and contraction level n=4. The polarizability of fluorine was adjusted in PIXEL to reproduce these data.

Figure ESI S1. The packing with orthogonal columns in the pyrene-1,4-benzoquinone cocrystal, PYRBZQ01 and the pyrene-chlorobenzoquinone cocrystal(CORPIJ)



PYRBZQ01 CORPIJ

Table ESI S4. Cocrystals of nitrobenzenss

APANBZ	1,3,5-trinitrobenzene - acepleiadylene
ASKNBZ	1,3,5-trinitrobenzene - acetylskatole
DBTTNB	1,3,5-trinitrobenzene - dibenzothiophene
VIGKIF	1,3,5-trinitrobenzene - chrysene
XAHZAH	1,3,5-trinitrobenzene - 1,3,5-triethynylbenzene
RUYLAY	1,3,5-trinitrobenzene - 1,10-phenanthroline
NIBJUF	1,3,5-trinitrobenzene - trinitrotoluene
PVVBFD01	1,3,5-trinitrobenzene - triphenylene
RUYKUR	1,3,5-trinitrobenzene - acridine
GEXMED	1,3,5-trinitrobenzene (bis[1,2,5]Oxadiazolo[3,4-e:3', 4'- g][2,1,3]benzoxadiazole 1,4,7-trioxide)
CECPEF	1,4-dinitrobenzene - 1,4diethynylbenzene
URIJEL	2,4,6-trinitrotoluene - anthracene
URIKEM	thieno[3,2-b]thiophene - 2,4,6-trinitrotoluene
URIKUC	4,6-dimethyldibenzothiophene - 2,4,6-trinitrotoluene
URILEN	1,4-dimethoxybenzene - 2,4,6-trinitrotoluene

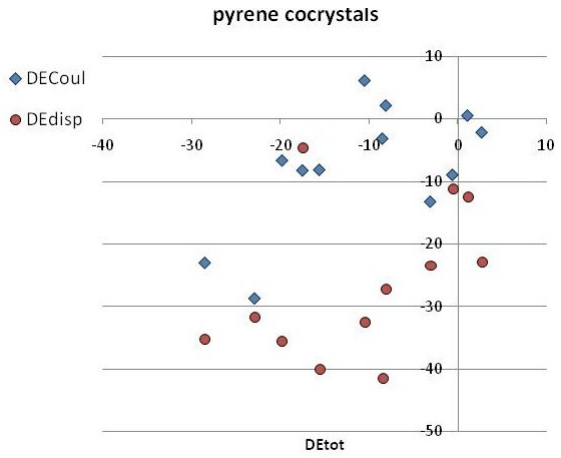


Figure ESI S2. The excess energies of cocrystal formation with pyrene. They are all stabilizing with a large dispersive contribution.

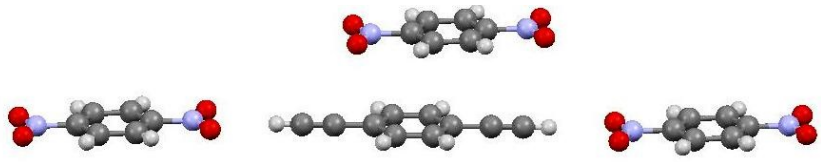


Figure ESI S3. The packing arrangement in 1,4-dinitrobenzene-1,4-diethynylbenzene (CECPEF), with ribbons of C-H...O bound molecules. This crystal has stabilizing bimolecular energies but destabilizing excess energies, Coulombic and dispersive (+10.3 and +26.5 kJ/mol respectively).

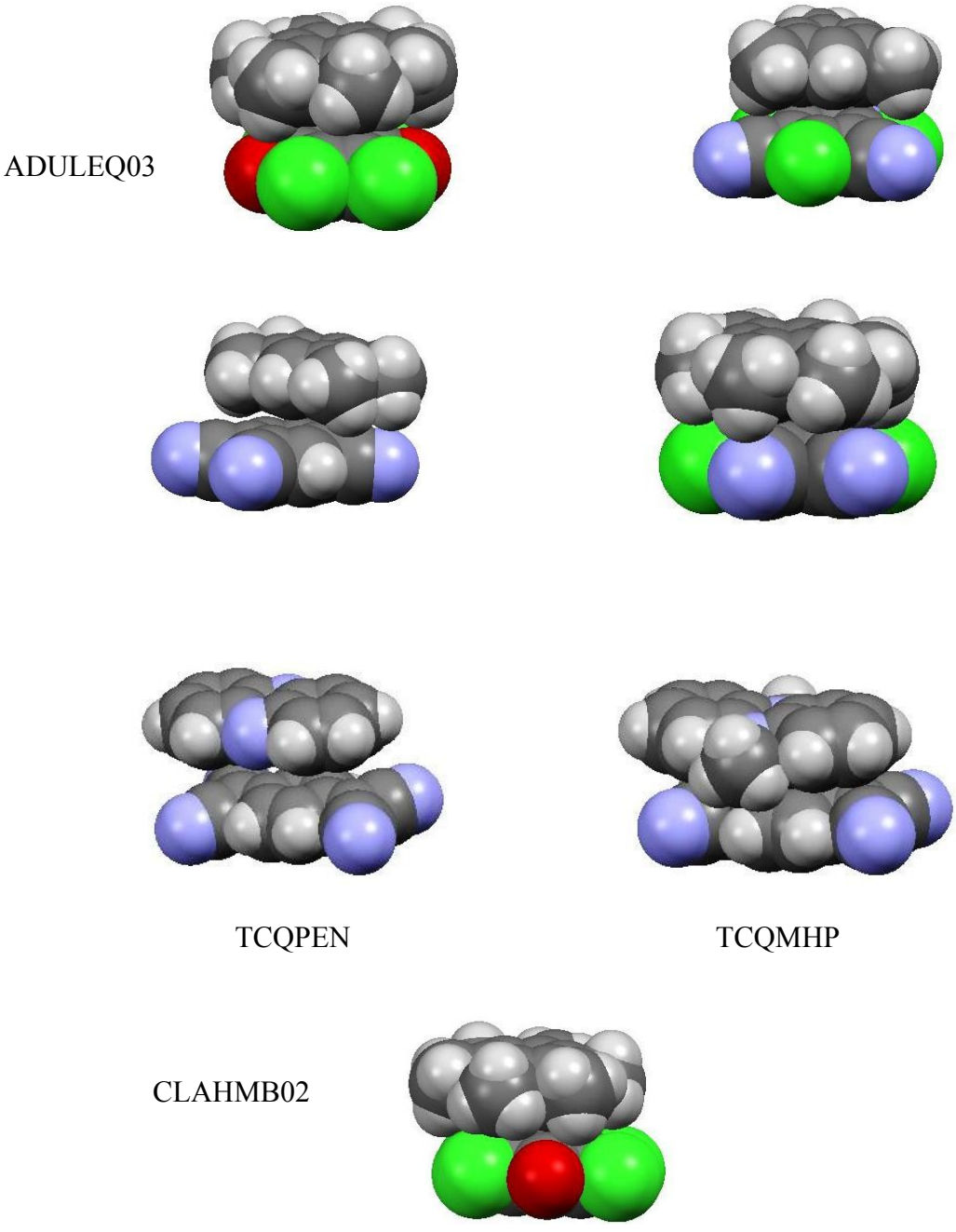


Figure ESI S4. A gallery of dimer stacked complexes with methylated hydrocarbons

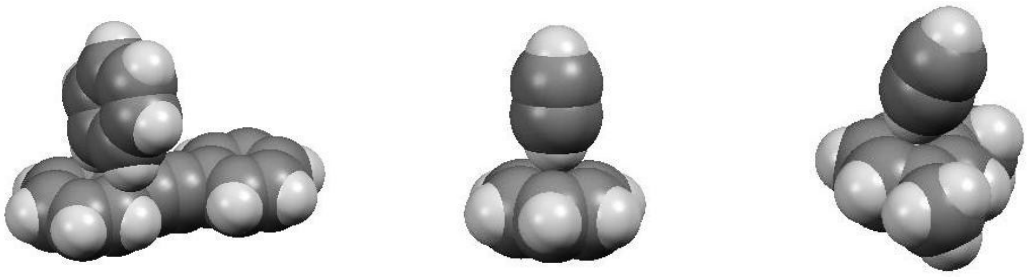


Figure ESI S5 . Cocrystals of hydrocarbons only: benzene-diphenylacetylene (KURCEG), benzene-acetylene (ELIQIZ), benzene m-xylene (GURNIR).

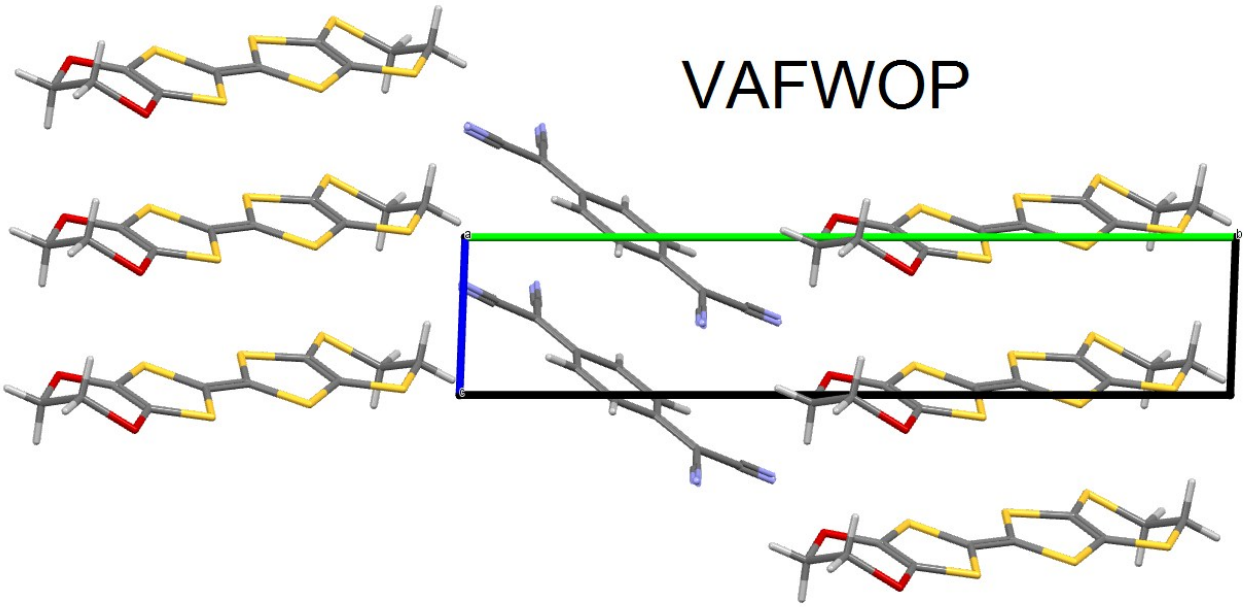


Figure ESI S6. VAFWOP cocrystal (Ethylenedioxyethylenedithiotetrathiafulvalene: 7,7,8,8-tetracyano-p-quinodimethane) as an example of unfavorable coupling energy (see text)

Table ESI S5. Ordered eigenvalues and relative amount of explained variance for each Principal Component in the Principal Component Analysis of the NOHB-ALL dataset (see the main text). Just the first 2 PC's satisfy the Kaiser-Guttman criterion of eigenvalue larger than unity (see the main text).

Principal component	Eigenvalue	Proportion (%)	Cumulative (%)
1	3.087548	51.46%	51.46%
2	1.121918	18.70%	70.16%
3	0.925917	15.43%	85.59%
4	0.538857	8.98%	94.57%
5	0.325758	5.43%	100.00%
6	0.000001	0.00%	100.00%

Table ESI S6. Unrotated factor loadings and amount of variance explained corresponding to the variables explored by means of the Principal Component Analysis of the the NOHB-ALL dataset (see the main text). E_{cx}, E_{cd}, E_{ce} and E_{cr} are the coupling energies (total, dispersive, electrostatic and repulsive). PE is the cocrystal packing energy and DV the difference of molecular volumes.

Attribute	PC1	Variance Explianed	PC2	Variance Explained
-	Corr.	% (Tot. %)	Corr.	% (Tot. %)
E_{cx}	-0.93962	88 % (88 %)	-0.07295	1 % (89 %)
E_{cd}	-0.92604	86 % (86 %)	-0.06366	0 % (86 %)
E_{cr}	0.80778	65 % (65 %)	-0.25221	6 % (72 %)
E_{ce}	-0.73926	55 % (55 %)	0.21931	5 % (59 %)
PE	-0.38195	15 % (15 %)	-0.71072	51 % (65 %)
DV	-0.04702	0 % (0 %)	0.70407	50 % (50 %)
Var. Expl.	3.08755	51 % (51 %)	1.12192	19 % (70 %)

Table ESI S7. Correlation matrix for variables employed to explain variance of the NOHB-ALL dataset (see the main text). E_{cx}, E_{cd}, E_{ce} and E_{cr} are the coupling energies (total, dispersive, electrostatic and repulsive). PE is the cocrystal packing energy and DV the difference of molecular volumes.

	E_{cx}	E_{cd}	E_{cr}	E_{ce}	PE	DV
E_{cx}	1.00000	0.89761	-0.57889	0.70504	0.36868	0.01371
E_{cd}	0.89761	1.00000	-0.75244	0.45226	0.37970	0.05486
E_{cr}	-0.57889	-0.75244	1.00000	-0.55129	-0.08849	-0.08929
E_{ce}	0.70504	0.45226	-0.55129	1.00000	0.04372	-0.00143
PE	0.36868	0.37970	-0.08849	0.04372	1.00000	-0.09585
DV	0.01371	0.05486	-0.08929	-0.00143	-0.09585	1.00000

Table ESI S8. Rotated factor loadings according with the VARIMAX technique (see A. Gavezzotti and L. Lo Presti, Crystal Growth & Design 16(5):2952-2962 for detailed information) of the variables employed to describe the NOHB-ALL dataset (see the main text). E_{cx}, E_{cd}, E_{ce} and E_{cr} are the coupling energies (total, dispersive, electrostatic and repulsive). PE is the cocrystal packing energy and DV the difference of molecular volumes. For each principal component, the corresponding eigenvalue is reported at the bottom of the column.

Axis →	PC1	PC2
E_{cx}	0.91640	0.22006
E_{cd}	0.90445	0.20875
E_{ce}	-0.83742	0.12181
E_{cr}	0.76458	-0.10012
PE	0.26522	0.76201
DV	0.15734	-0.68787
Var. Expl.	3.03877	1.1707