Supplementary Material

Examining the Role of Molecular and Crystallographic Symmetry in Isomorphism: A Series of Centrosymmetric "Bridge-Flipped" Trifluoromethyl-Substituted *bis*-Benzylideneanilines

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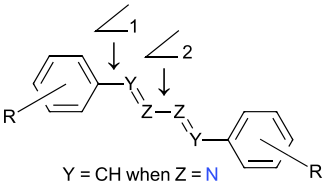
Table S1. Angles between least-squares planes: Published *hyd/gly* isomers



Y = CH when Z = N

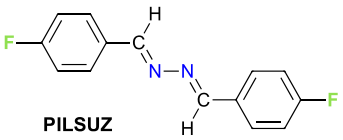
Y = N when Z = CH

1 = angle (°) between ring plane and adjacent HC=N plane

2 = angle (°) between HC=N planes (zero for molecule on center)

3 = angle (°) between ring planes (zero for molecule on center)

No Isomorphous Pairs

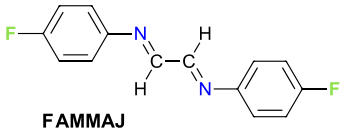


PILSUZ

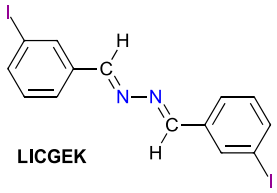
1 = 3.73 / 19.47

2 = 0 / 0

3 = 0 / 0



FAMMAJ

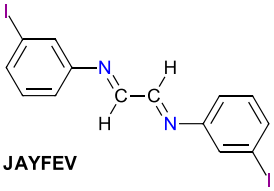


LICGEK

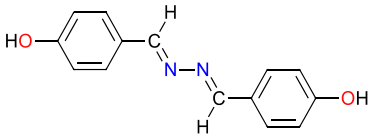
1 = 11.65 / 7.45

2 = 0 / 0

3 = 0 / 0



JAYFEV



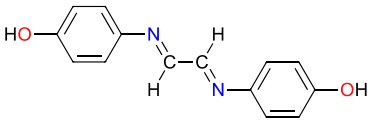
CICRUC/CICRUC01

not on center

1 = 4.08, 8.58 / 22.76

2 = 16.52 / 0

3 = 11.97 / 0

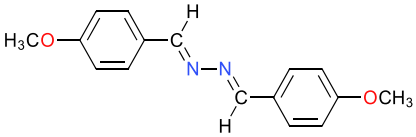


AGOYAZ

1 = 0.54, 5.93 / 27.70

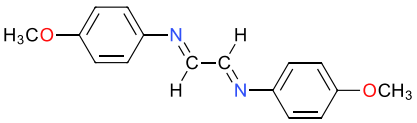
2 = 4.22 / 0

3 = 8.83 / 0



ANISAZ/ANISAZ01-04, 06, 07, 09

not on center

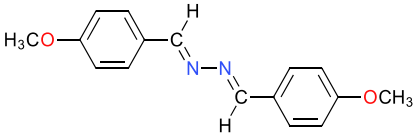


DIRJUN

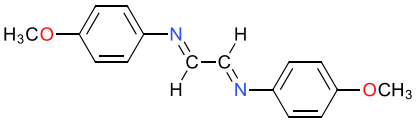
1 = 4.66, 8.39 / 27.70

2 = 0, 0 / 0

3 = 0, 0 / 0



ANISAZ05

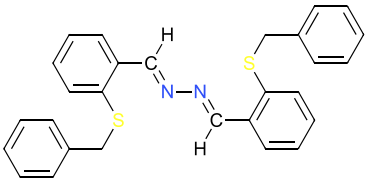


DIRJUN

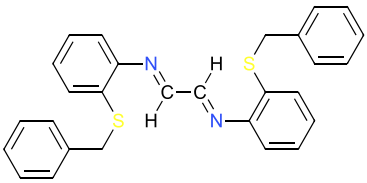
1 = 12.15 / 33.95

2 = 0 / 0

3 = 0 / 0



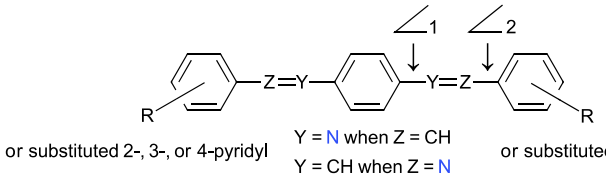
ODANEN



YOPWOT

Table S2. Angles between least-squares planes:

Published *phe/ter* isomers



or substituted 2-, 3-, or 4-pyridyl Y = N when Z = CH; Y = CH when Z = N or substituted 2-, 3-, or 4-pyridyl

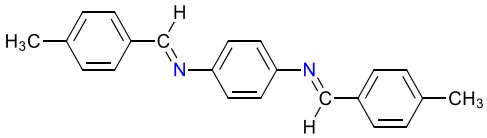
1 = angle (°) between center ring plane and HC=N plane

2 = angle (°) between terminal ring plane and HC=N plane

3 = angle (°) between center ring plane and terminal ring plane

4 = angle (°) between terminal ring planes (zero for molecule on center)

Isomorphous Pairs

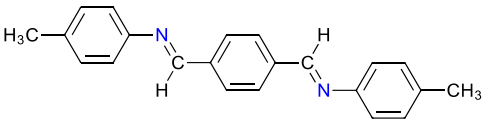


YAGSEG/YAGSEG01

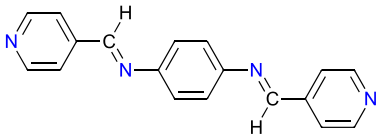
1 = 42.43 / 11.10

2 = 4.43 / 12.03

3 = 46.64 / 2.45



WILSOZ/WILSOZ01/WILSOZ02

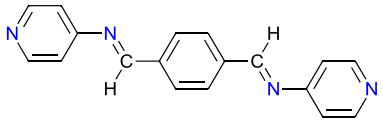


PEXXEW/PEXXEW01-06

1 = 46.28, 48.75 / 6.36, 8.85

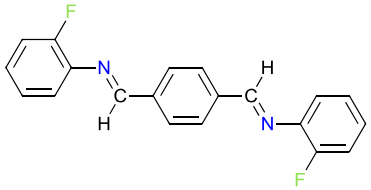
2 = 7.24, 9.55 / 40.26, 54.83

3 = 53.29, 58.10 / 46.62, 63.65



MINWIS

Nonisomorphous Pairs

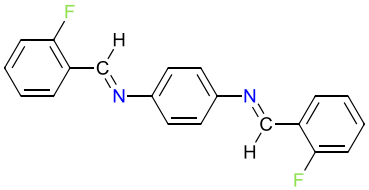


WIXSAZ/WIXSAZ01

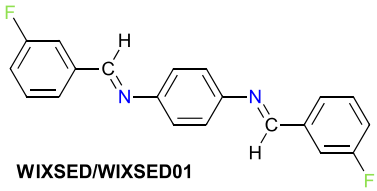
1 = 19.73 / 12.53

2 = 5.55 / 41.29

3 = 15.10 / 53.42



WIXRIG/WIXRIG01

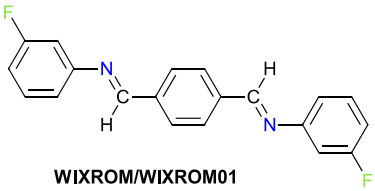


WIXSED/WIXSED01

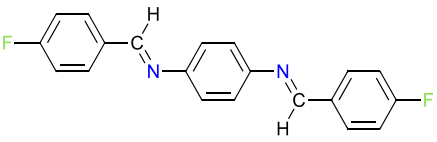
1 = 29.69 / 5.22

2 = 15.95 / 42.26

3 = 14.09 / 47.45



WIXROM/WIXROM01



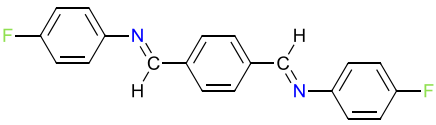
HEWHAU

1 = 38.90, 39.77 / 13.70, 14.11

2 =13.45, 14.56 / 38.80, 37.65

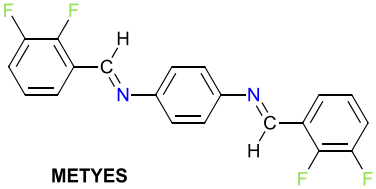
3 = 52.19, 54.33 / 52.47, 51.42

4 = 0 / 3.64



HEWHAU01/QIYQIA/QIYQIA01

not on center s-*cis*

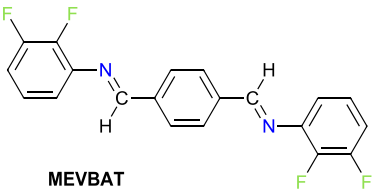


METYES

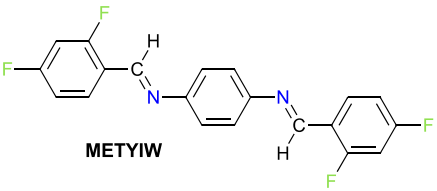
1 = 18.14 / 2.19

2 = 4.53 / 43.52

3 = 14.63 / 41.52



MEVBAT

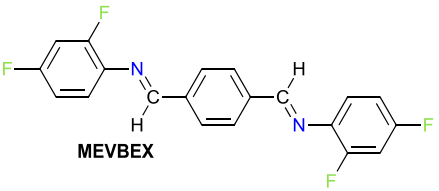


METYIW

1 = 20.78 / 1.84

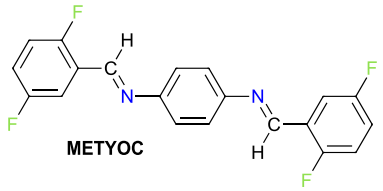
2 = 4.36 / 20.04

3 = 17.52 / 21.81



MEVBEX

Table S2 (continued)

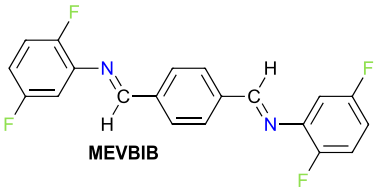


METYOC

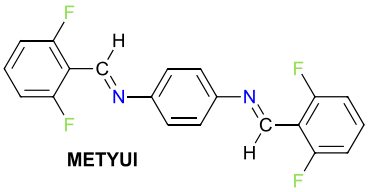
1 = 39.12 / 2.91, 3.22

2 = 2.95 / 38.92, 41.14

3 = 41.87 / 36.69, 37.93



MEVBIB

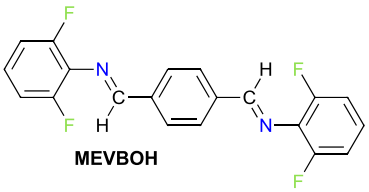


METYUI

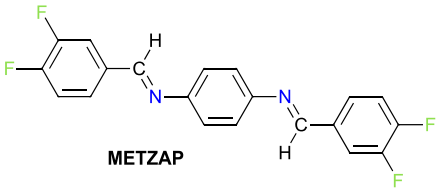
1 = 36.32 / 3.58

2 = 5.57 / 46.97

3 = 41.20 / 50.17



MEVBOH

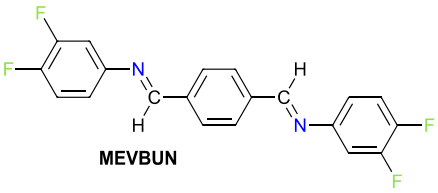


METZAP

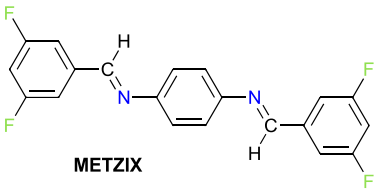
1 = 41.99 / 4.14

2 = 2.06 / 4.90

3 = 43.85 / 1.30



MEVBUN

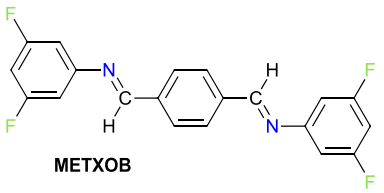


METZIX

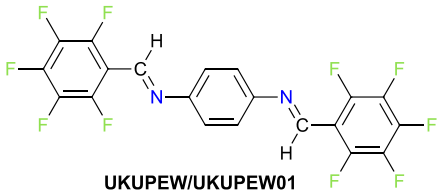
1 = 23.49, 36.35 / 1.16

2 = 14.09, 4.15 / 40.62

3 = 10.20, 40.11 / 39.47



METXOB

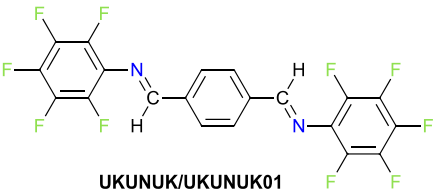


UKUPEW/UKUPEW01

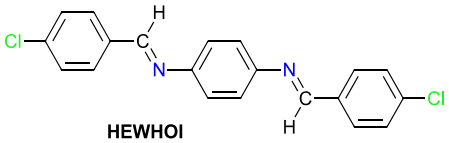
1 = 13.82 / 3.58

2 = 10.71 / 39.28

3 = 3.82 / 35.98



UKUNUK/UKUNUK01

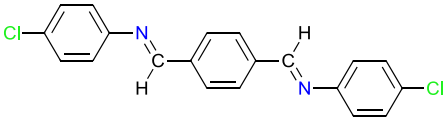


HEWHOI

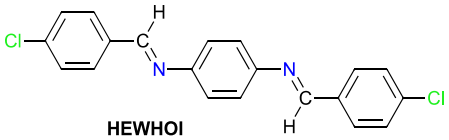
1 = 13.17, 15.30 / 3.64, 8.52

2 = 6.88, 10.67 / 7.70, 17.56

3 = 7.62, 5.19 / 4.47, 9.84



QIYQOG

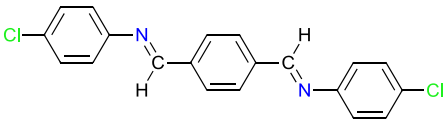


HEWHOI

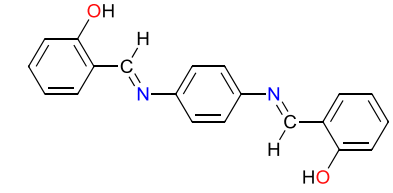
1 = 13.17, 15.30 / 2.43

2 = 6.88, 10.67 / 49.41

3 = 7.62, 5.19 / 47.94



QIYQOG01

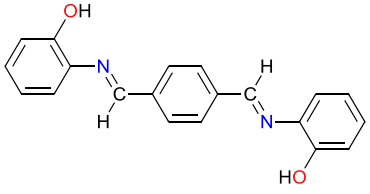


EJUVOW/KIWCUR/SANYIP/SANYIP01-03

1 = 4.49 / 13.39

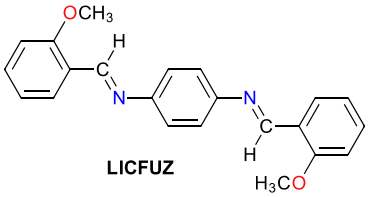
2 = 1.93 / 6.76

3 = 3.58 / 7.29



XIGRIO/XIGRIO01

Table S2 (continued)

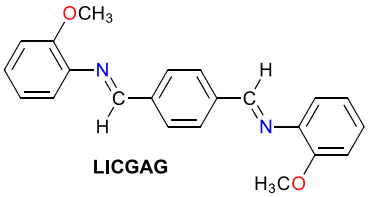


LICFUZ

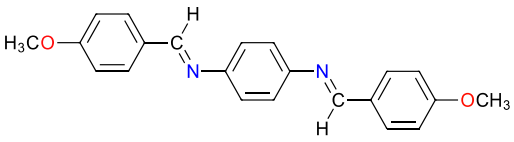
1 = 18.05 / 1.52

2 = 6.36 / 44.77

3 = 12.15 / 46.28



LICGAG



HEWGUN

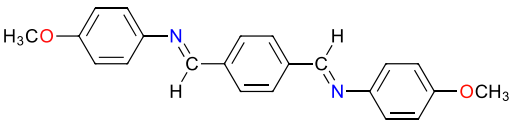
not on center s-*trans*

1 = 17.11, 23.84 / 8.94

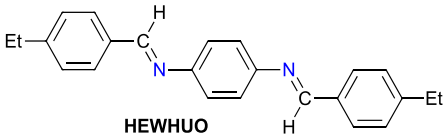
2 = 8.80, 10.73 / 22.01

3 =8.69, 13.49 / 13.13

4 =4.85 / 0



QIYSUO/QIYSUO01



HEWHUO

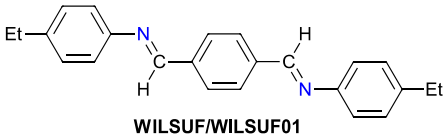
two molecules not on centers s-*cis*

1 = 48.43, 50.86 ; 46.95, 45.99 / 1.24

2 = 14.43, 14.53 ; 15.26, 14.14 / 34.56

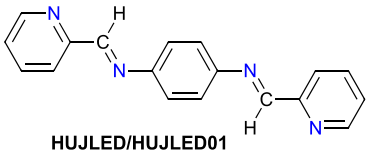
3 = 62.52, 65.16 ; 61.96, 59.88 / 33.57

4 = 53.14 ; 58.47 / 67.15



WILSUF/WILSUF01

on twofold axis s-*trans*



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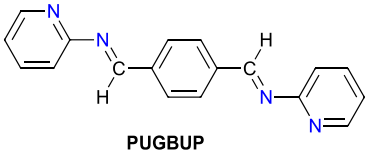
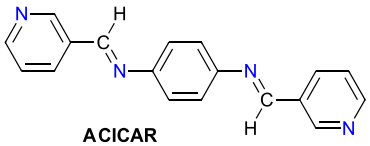
1 = 15.18 / 1.45

2 = 3.27 / 3.00

3 = 11.93 / 2.70



PUGBUP



ACICAR

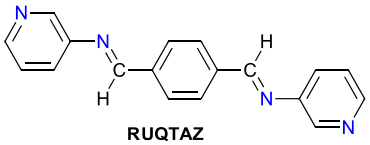
not on center s-*trans*

1 = 1.24, 2.47 / 1.04

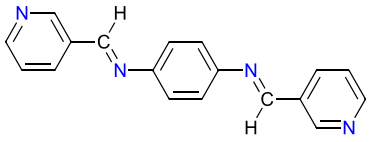
2 = 1.11, 0.67 / 42.21

3 = 1.69, 1.88 / 42.53

4 = 0.36 / 0



RUQTAZ

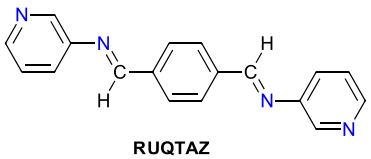


ACICAR01

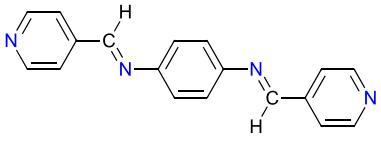
1 = 36.07 / 1.04

2 = 4.22 / 42.21

3 = 31.88 / 42.53



RUQTAZ

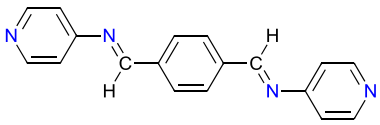


PEXXEW/PEXXEW01-06

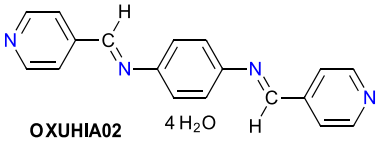
1 = 46.28, 48.75 / 4.62

2 = 7.24, 9.55 / 43.97

3 = 53.29, 58.10 / 48.57



MINWIS01

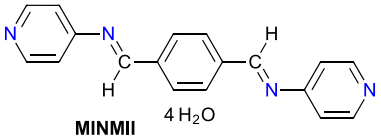


OXUHIA02 4 H_2O

1 = 44.23 / 3.42

2 = 8.26 / 44.89

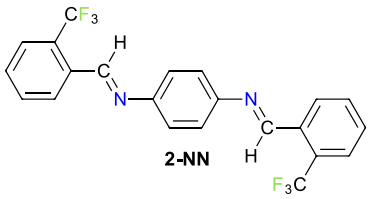
3 = 52.49 / 41.48



MINMII 4 H_2O

Table S2 (continued)

phe/ter isomers reported in this work



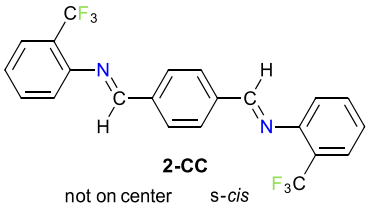
2-NN

1 = 31.60 / 5.76, 2.98

2 = 6.62 / 57.18, 27.01

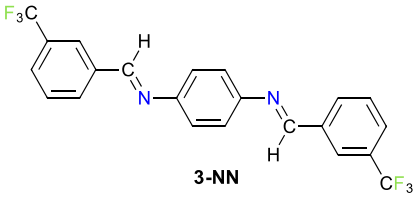
3 = 26.01 / 62.62, 29.00

4 = 0 / 88.61



2-CC

not on center s-*cis*

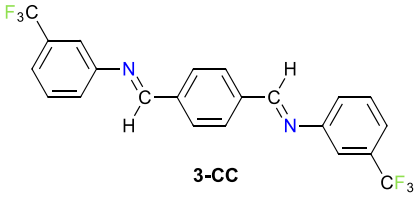


3-NN

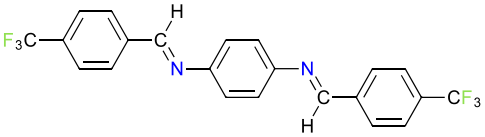
1 = 10.27 / 0.97

2 = 3.77 / 7.05

3 = 6.51 / 8.01



3-CC



4-NN

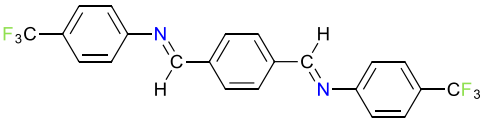
HEWHIC

1 = 38.62 / 6.00, 13.72

2 = 2.38 / 41.56, 39.36

3 = 40.62 / 47.57, 52.81

4 = 0 / 9.96



4-CC

not on center s-*trans*

Table S3. Intermolecular approaches involving F atoms

		F···H (Å)	C-F···H (°)	F···H-C (°)		
2-NN	C11-F3···H6-C6^{i}	2.61	111	140		
2-CC	C22-F4···H5-C5^{ii}	2.65	145	126		
	C22-F5···H3-C3^{iii}	2.59	131	124		
			F···Cg (Å)	**C-F···Cg (°)**		
	C22-F6···Cg(1)^{iv}		3.4590(15)	144.20(10)		
3-NN	C11-F2···H4-C4^{v}	2.50	167	171		
	C11-F3…H2-C2^{vi}	2.40	134	168		
3-CC	C11-F1···H10-C10^{vi}	2.52	170	155		
	C11-F2···H4-C4^{v}	2.56	162	157		
	C11-F3···H2-C2^{vi}	2.62	130	155		
4-NN*	C1-F1···H8-C8^{vii}	2.56	169	163		
	C1-F1'···H6-C6^{viii}	2.52	150	118		
	C1-F2···H7-C7^{ix}	2.49	169	161		
			F···F (Å)	**C-F···F (°)**	**F···F-C (°)**	
	C1-F3···F3-C1^{x}		2.800(3)	164.5(2)	164.5(2)	
			F···Cg (Å)	**C-F···Cg (°)**		
	C1-F3'···Cg(2)^{xi}		3.033(19)	141.9(13)		
			F···F (Å)	**C-F···F (°)**	**F···F-C (°)**	
4-CC*	C21-F3···F4'-C22' ^{xii}		2.867(11)	100.2(3)	99.8(7)	
	C22-F4···H5-C5^{xiii}	2.42	120	144		
	C22-F5···H16-C16^{xiv}	2.59	113	132		
			F···Cg (Å)	**C-F···Cg (°)**		
	C22'-F5'···Cg(3)^{xv}		3.422(13)	143.3(6)		

*disordered CF_3 groups

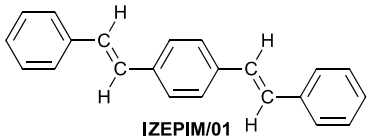
Cg(1) = centroid of C1-C2-C3-C4-C5-C6

Cg(2) = centroid of C2-C3-C4-C5-C6-C7

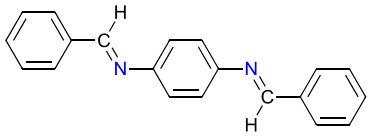
Cg(3) = centroid of C11-C12-C13-C14-C15-C16

symmetry codes: i = -1/2-x,-1/2+y,1/2-z ; ii = 2-x,-y,1-z ; iii = 1-x,-y,1-z ; iv = -1/2+x,1/2-y,1/2+z ; v = 1-x, -2-y, 2-z ; vi = 1/2-x, -1/2+y, 3/2-z ; vii = 1+x, -1+y, z; viii = x, -1+y, z ; ix = 2-x, -y, -z ; x = 1-x, -1-y, -z ; xi = 1+x, y, z ; xii = -3/2+x, 3/2-y, -1/2+z ; xiii = 3/2-x, -1/2+y, 1/2-z ; xiv = 5/2-x, 1/2+y, 1/2-z ; xv = 5/2-x, -1/2+y, 1/2-z

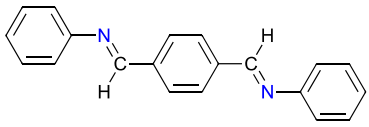
Table S4. Published *bis*-styryl, *bis*-benzylidene, and *bis*-azo series



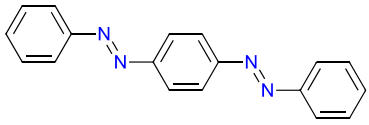
IZEPIM/01
IZEPIM02
both unique



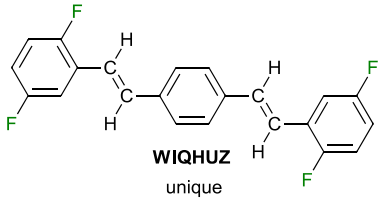
(not reported in CSD)



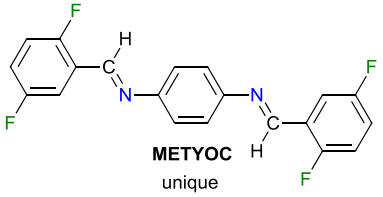
WILSIT/01/02/03/04
unique



PHDAZB10
unique



WIQHUZ
unique



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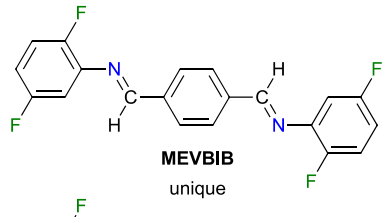

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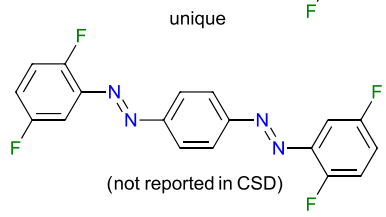

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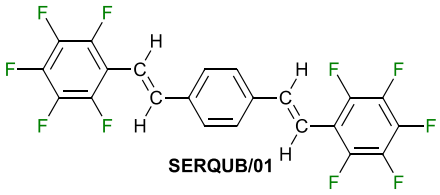
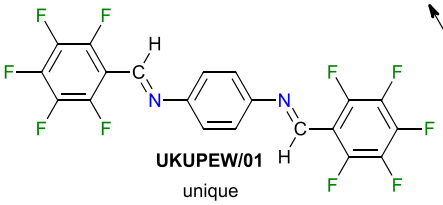
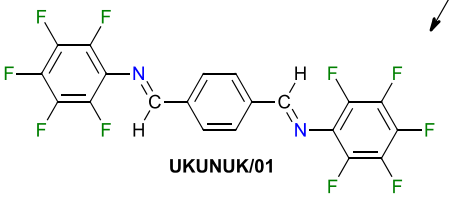


SERQUB/01

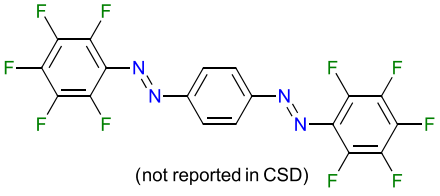


UKUPEW/01
unique

isomorphous



UKUNUK/01



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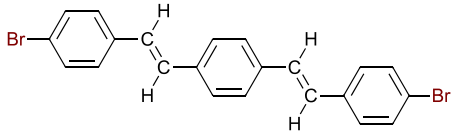

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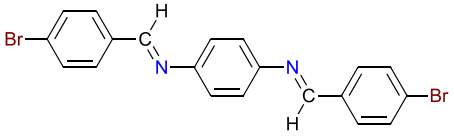

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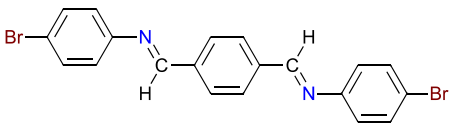

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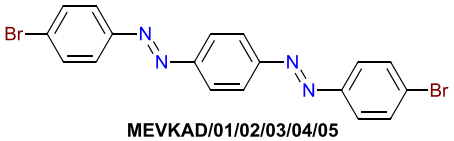

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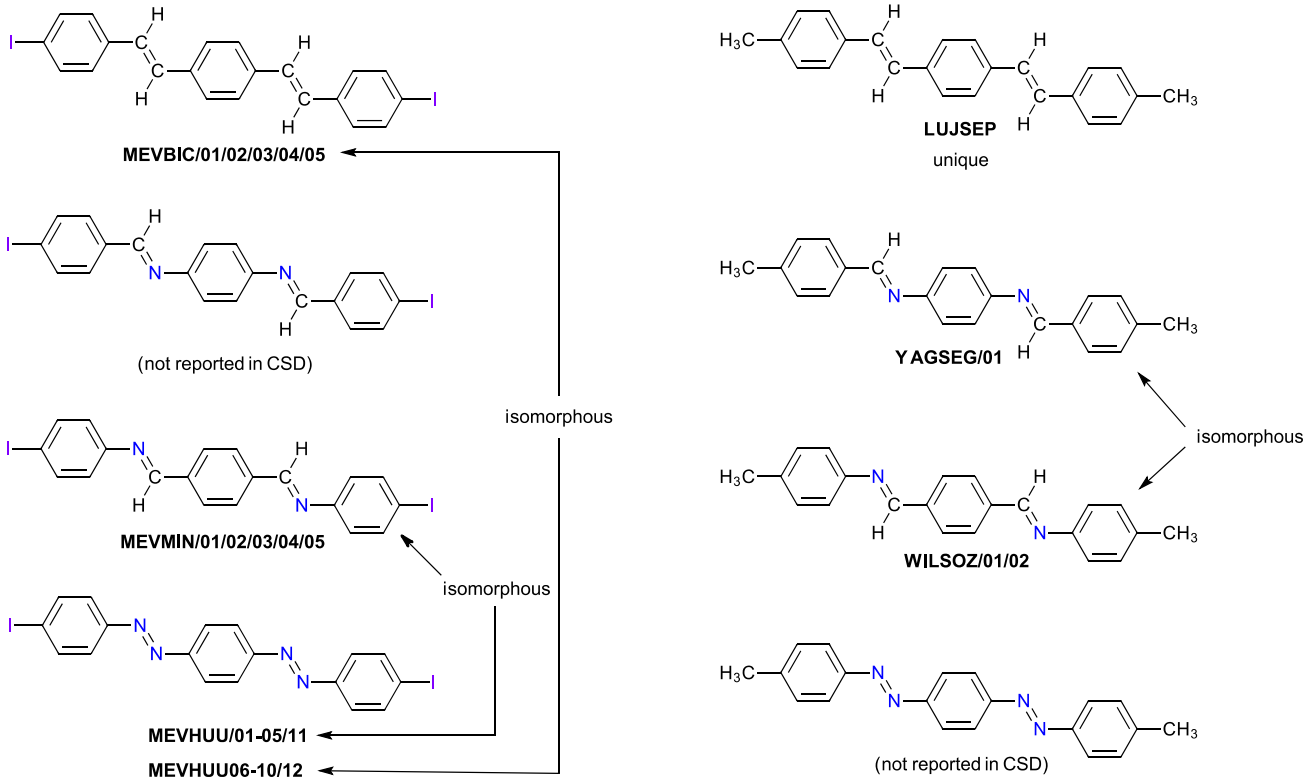


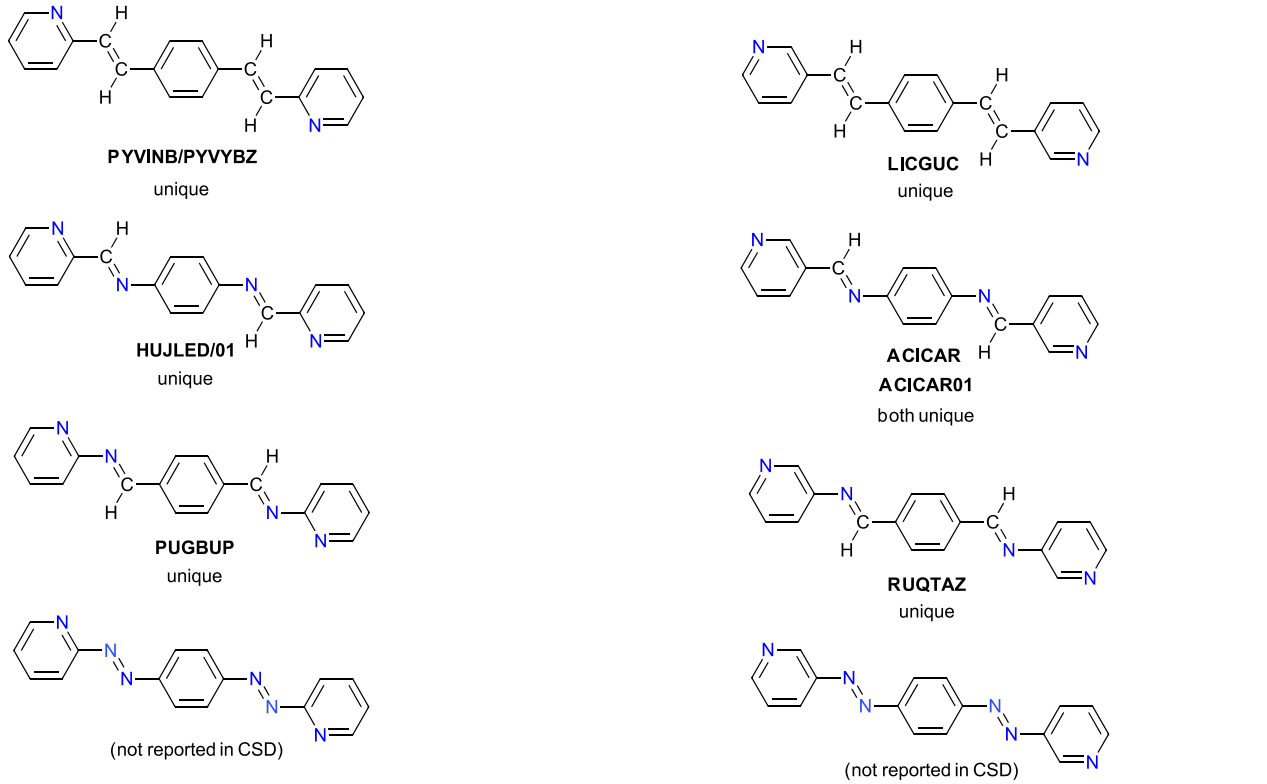
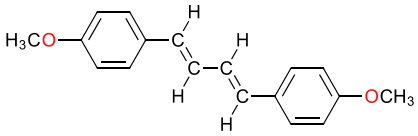
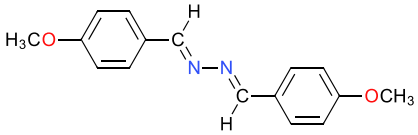


Table S5. An extended *hyd/gly* series.

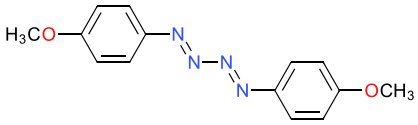


KABKAB
unique



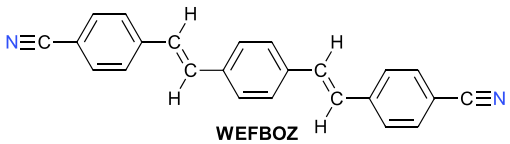
ANISAZ/ANISAZ01-04, 06, 07, 09
ANISAZ05
both unique

DIRJUN
unique

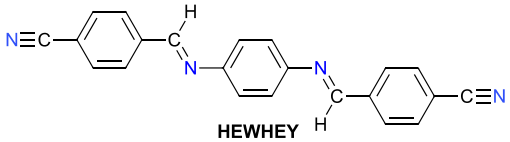


(not reported in CSD)

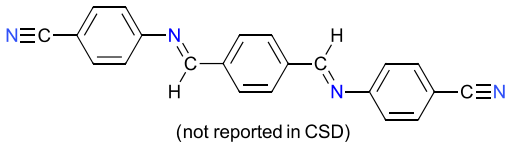
Table S6. Series with one unsymmetrical spacer



WEFBOZ
unique



HEWHEY
unique



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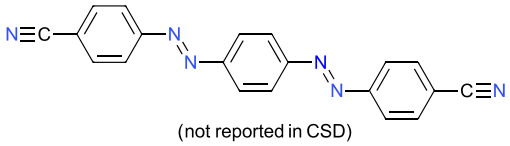

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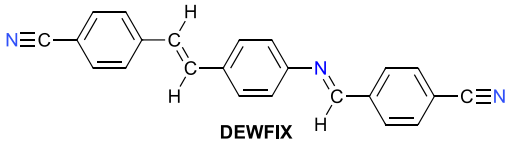


DEWFIX
unique

Supplementary Materials References

(structures used for planes calculations are indicated by underlined refcodes)

Table S1

PILSUZ: M. Odabasoglu, O. Buyukgungor, K. Sunil, B. Narayana, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2007, **63**, o4145-o4146.

FAMMAJ: D. A. J. Harding, E. G. Hope, K. Singh, G. A. Solan, *Polyhedron*, 2012, **33**, 360-366.

LICGEK: W. H. Ojala, T. M. Arola, N. Herrera, B. Balidemaj, C. R. Ojala, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2007, **63**, o207-o211.

JAYFEV: H. M. Cho, J. S. Moore, S. R. Wilson, *Acta Crystallogr. Sect. E: Struct. Rep. Online*, 2005, **61**, o3773-o3774.

CICRUC: G. Liu, L. Xie, Y. Wang, J.-D. Wang, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2007, **63**, o2611.

CICRUC01: T. G. D. van Schalkwyk, A. M. Stephen, *ARKIVOC*, 2005, **2005**, 109-8.

AGOYAZ: L. Biancalana, S. Fulignati, C. Antonetti, S. Zacchini, G. Provinciali, G. Pampaloni, A. M. R. Galletti, F. Marchetti, *New J. Chem*, 2018, **42**, 17574-17586.

ANISAZ: J.-L. Galigne, J. Falgueirettes, *Acta Crystallogr.,Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1968, **24**, 1523-1529.

ANISAZ01: H. Astheimer, L. Walz, W. Haase, J. Loub, H. J. Muller, M. Gallardo, *Mol. Cryst. Liq. Cryst.,* 1985, **131**, 343-351.

ANISAZ02: S. V. Sereda, M. Yu. Antipin, T. V. Timofeeva, Yu.T. Struchkov, *Kristallografiya*, 1988, **33**, 118

ANISAZ03: S. Lakshmi, M. A. Sridhar, J. Shashidhara Prasad, J. Indira, P. P. Karat, B. Veerendra, B. Shivarama Holla, *Mol. Cryst. Liq. Cryst.*, 2002, **381**, 59-68.

ANISAZ04: B. Narayana, H. S. Yathirajan, B. K. Sarojini, M. Bolte, *CSD Communication*, 2007.

ANISAZ05: J.-Y. Jin, K. Zhang, L.-X. Zhang, A.-J. Zhang, Y.-Z. Liu, *Z. Kristallogr. - New Cryst. Struct.*, 2007, **222**, 391-392.

ANISAZ06: J. T. Mague, S. K. Mohamed, *CSD Communication*, 2016.

ANISAZ07: B. F. Abdel-Wahab, M. H. Alotaibi, G. A. El-Hiti, *CSD Communication*, 2017.

ANISAZ09: L. R. Gomes, J. N. Low, N. R. de L. Correira, T. C. M. Noguiera, A. C. Pinheiro, M. V. N. de Souza, J. L. Wardell, S. M. S. V. Wardell, *Z. Kristallogr. – Cryst. Mat.*, 2019, **234**, 59-71.

DIRJUN: E. Higgins, A. C. O'Donoghue, D. S. Yufit, J. A. K. Howard, *CSD Communication*, 2023.

ODANEN: C. G. Hamaker, B. P. Oberts, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2006, **62**, o1780-o1781.

YOPWOT: K. Merzweiler, *CSD Communication*, 2024.

Table S2

YAGSEG: H. Li, Y. Xiang, H. Han, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2011, **67**, o2953.

YAGSEG01: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

WILSOZ: W. Thyen, P. Zugenmaier, *Cryst. Res. Technol.,* 1994, **29**, 449-456.

WILSOZ01: P. Zugenmaier, *Int. J. Mol. Sci.*, 2011, **12**, 7360-7400.

WILSOZ02: Z. Fang, C. Cao, J. Chen, X. Deng, *J. Mol. Struct.*, 2014, **1063**, 307-312.

PEXXEW: Q.-F. Hou, L. Ye, S.-M. Jiang, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2007, **63**, o939-o940.

PEXXEW01-06: N. Juneja, D. K. Unruh, G. C. George III, K. M. Hutchins, *Cryst. Growth Des.*, 2022, **23**, 524-531.

MINWIS: R. Sanii, A. Bajpai, E. Patyk-Kaźmierczak, M. J. Zaworotko, *ACS Sustainable Chem. Eng.*, 2018, **6**, 14589-14598.

WIXSAZ: W. H. Ojala, B. Balidemaj, J. A. Johnson, S. N. Larson, C. R. Ojala, *CrystEngComm*, 2014, **16**, 7226-7235.

WIXSAZ01: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

WIXRIG: W. H. Ojala, B. Balidemaj, J. A. Johnson, S. N. Larson, C. R. Ojala, *CrystEngComm*, 2014, **16**, 7226-7235.

WIXRIG01: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

WIXSED: W. H. Ojala, B. Balidemaj, J. A. Johnson, S. N. Larson, C. R. Ojala, *CrystEngComm*, 2014, **16**, 7226-7235.

WIXSED01: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

WIXROM: W. H. Ojala, B. Balidemaj, J. A. Johnson, S. N. Larson, C. R. Ojala, *CrystEngComm*, 2014, **16**, 7226-7235.

WIXROM01: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

HEWHAU: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

HEWHAU01: W. H. Ojala, B. Balidemaj, J. A. Johnson, S. N. Larson, C. R. Ojala, *CrystEngComm*, 2014, **16**, 7226-7235.

QIYQIA: Z. Fang, C. Cao, J. Chen, X. Deng, *J. Mol. Struct.*, 2014, **1063**, 307-312.

QIYQIA01: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METYES: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

MEVBAT: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METYIW: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

MEVBEX: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METYOC: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

MEVBIB: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METYUI: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

MEVBOH: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METZAP: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

MEVBUN: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METZIX: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

METXOB: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

UKUPEW: A. Collas, R. De Borger, T. Amanova, F. Blockhuys, *CrystEngComm*, 2011, **13**, 702-710.

UKUPEW01: W. Pang, J.-W. Zhao, L. Zhao, Z.-K. Zhang, S.-Z. Zhu, *J. Mol. Struct. Struct.,* 2015, **1096**, 21-28.

UKUNUK: A. Collas, R. De Borger, T. Amanova, F. Blockhuys, *CrystEngComm*, 2011, **13**, 702-710.

UKUNUK01: W. Pang, J.-W. Zhao, L. Zhao, Z.-K. Zhang, S.-Z. Zhu, *J. Mol. Struct. Struct.,* 2015, **1096**, 21-28.

HEWHOI: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

QIYQOG: Z. Fang, C. Cao, J. Chen, X. Deng, *J. Mol. Struct.*, 2014, **1063**, 307-312.

QIYQOG01: K. J. Rajimon, A. Y. Alzahrani, D. S. R. Nair, D. P. Venkatesh, R. Thomas, *J. Mol. Struct.*, 2024, **1312**, 138546.

EJUVOW: C. Niu, L. Zhao, T. Fang, X. Deng, H. Ma, J. Zhang, N. Na, J. Han, and J. Ouyang, *Langmuir*, 2014, **30**, 2351-2359.

KIWCUR: S. Guieu, F. Cardona, J. Rocha, A. M. S. Silva, *Chem. Eur. J.*, 2018, **24**, 17262-17267.

SANYIP: N. Hoshino, T. Inabe, T. Mitani, Y. Maruyama, *Bull. Chem. Soc. Jpn.*, 1988, **61**, 4207-4214.

SANYIP01: T. Inabe, N. Hoshino, T. Mitani, Y. Maruyama, *Bull. Chem. Soc. Jpn.*, 1989, **62**, 2245-2251.

SANYIP02: S. Zhang, S. Ye, T. Zhang, X. Li, *Chem. Res. Chin. Univ.*, 2004, **20**, 562.

SANYIP03: J. T. Mague, S. K. Mohamed, *CSD Communication*, 2024.

XIGRIO: S. Chakraborty, R. H. Laye, R. L. Paul, R. G. Gonnade, V. G. Puranik, M. D. Ward, G. K. Lahiri, *J. Chem. Soc., Dalton Trans.*, 2002, 1172-1179.

XIGRIO01: P. Torawane, K. Keshav, M. K. Kumawat, R. Srivastava, T. Anand, S. Sahoo, A. Borse, A. Kuwar, *Photochem. Photobiol. Sci.*, 2017, **16**, 1464-1470.

LICFUZ: W. H. Ojala, T. M. Arola, N. Herrera, B. Balidemaj, C. R. Ojala, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2007, **63**, o207-o211.

LICGAG: W. H. Ojala, T. M. Arola, N. Herrera, B. Balidemaj, C. R. Ojala, *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.*, 2007, **63**, o207-o211.

HEWGUN: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

QIYSUO: Z. Fang, C. Cao, J. Chen, X. Deng, *J. Mol. Struct.*, 2014, **1063**, 307-312.

QIYSUO01: Z.-Q. Liu, M. G. Tay, E. Enggie, *CSD Communication*, 2016.

HEWHUO: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

WILSUF: W. Thyen, P. Zugenmaier, *Cryst. Res. Technol.,* 1994, **29**, 449-456.

WILSUF01: P. Zugenmaier, *Int. J. Mol. Sci.*, 2011, **12**, 7360-7400.

HUJLED: N. Chanda, B. Mondal, V. G. Puranik, G. K. Lahiri, *Polyhedron*, 2002, **21**, 2033-2043.

HUJLED01: P. J. Ball, T. R. Shtoyko, J. A. K. Bauer, W. J. Oldham, W. B. Connick, *Inorg. Chem.*, 2004, **43**, 622-632.

PUGBUP: L.-H. Huo, S. Gao, S. W. Ng, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2009, **65**, o2659.

ACICAR: H. N. Kim, H. K. Lee, S. W. Lee, *Bull. Korean Chem. Soc.*, 2005, **26**, 892-898.

ACICAR01: K. Ha, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2011, **67**, o2250.

RUQTAZ: V. Stilinovic, D. Cincic, B. Kaitner, *Acta Chim. Slov.*, 2008, **55**, 874.

MINWIS01: R. Sanii, A. Bajpai, E. Patyk-Kaźmierczak, M. J. Zaworotko, *ACS Sustainable Chem. Eng.*, 2018, **6**, 14589-14598.

OXUHIA02: A. Bajpai, H. S. Scott, T. Pham, K.-J. Chen, B. Space, M. Lusi, M. L. Perry, M. J. Zaworotko, *IUCrJ*, 2016, **3**, 430-439.

MINMII: R. Sanii, A. Bajpai, E. Patyk-Kaźmierczak, M. J. Zaworotko, *ACS Sustainable Chem. Eng.*, 2018, **6**, 14589-14598.

HEWHIC: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

Table S4

IZEPIM: C. C. Wu, M. C. DeLong, Z. V. Vardeny, J. P. Ferraris, J. J. Gutierrez, *Synth. Met.*, 2003, **137**, 939-941.

IZEPIM01: S. Varghese, S. K. Park, S. Casado, R. C. Fischer, R. Resel, B. Milian-Medina, R. Wannemacher, S. Y. Park, J. Gierschner, *J. Phys. Chem. Lett.* 2013, **4**, 1597-1602.

IZEPIM02: D. Zhang, J. De, Y. Lei, H. Fu, *Nat. Comm.* 2021, **12**, 1838.

WILSIT: W. Thyen, P. Zugenmaier, *Cryst. Res. Technol.,* 1994, **29**, 449-456.

WILSIT01: P. Zugenmaier, *Int. J. Mol. Sci.*, 2011, **12**, 7360-7400.

WILSIT02: Z. Fang, C. Cao, J. Chen, X. Deng, *J. Mol. Struct.*, 2014, **1063**, 307-312.

WILSIT03: L. Wei, X. Hai, T. Xu, Z. Wang, W. Jiang, S. Jiang, Q. Wang, Y.-B. Zhang, Y. Zhao, *Nat. Commun.*, 2024, **15**, 2411.

WILSIT04: S. Liu, L. Wei, T. Zeng, W. Jiang, Y. Qiu, X. Yao, Q. Wang, Y. Zhao, Y.-B. Zhang, *J. Am. Chem. Soc.*, 2024, 146, 34053-34063.

PHDAZB10: R. D. Gilardi, I. L. Karle, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1972, **28**, 1635-1638.

WIQHUZ: M. L. Renak, G. P. Bartholomew, S. Wang, P. J. Ricatto, R. J. Lachicotte, G. C. Bazan, *J. Am. Chem. Soc.*, 1999, **121**, 7787-7799.

METYOC: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

MEVBIB: S. Dhingra, D. J. Barman, H. R. Yadav, J. Eyyathiyil, P. Bhowmik, P. Kaur, D. Adhikari, A. R. Choudhury, *CrystEngComm*, 2018, **20**, 716-727.

SERQUB: G. W. Coates, A. R. Dunn, L. M. Henling, J. W. Ziller, E. B. Lobkovsky, R. H. Grubbs, *J. Am. Chem. Soc.*, 1998, **120**, 3641-3649.

SERQUB01: M. L. Renak, G. P. Bartholomew, S. Wang, P. J. Ricatto, R. J. Lachicotte, G. C. Bazan, *J. Am. Chem. Soc.*, 1999, **121**, 7787-7799.

UKUPEW: A. Collas, R. De Borger, T. Amanova, F. Blockhuys, *CrystEngComm*, 2011, **13**, 702-710.

UKUPEW01: W. Pang, J.-W. Zhao, L. Zhao, Z.-K. Zhang, S.-Z. Zhu, *J. Mol. Struct. Struct.,* 2015, **1096**, 21-28.

UKUNUK: A. Collas, R. De Borger, T. Amanova, F. Blockhuys, *CrystEngComm*, 2011, **13**, 702-710.

UKUNUK01: W. Pang, J.-W. Zhao, L. Zhao, Z.-K. Zhang, S.-Z. Zhu, *J. Mol. Struct. Struct.,* 2015, **1096**, 21-28.

MEVCOJ/01/02/03/04/05: X. Ding, E. Zahid, D. K. Unruh, K. M. Hutchins , *IUCrJ*, 2022, **9**, 31-42.

METZEU/01/02/03/04/05: X. Ding, E. Zahid, D. K. Unruh, K. M. Hutchins , *IUCrJ*, 2022, **9**, 31-42.

MEVKAD/01/02/03/04/05: X. Ding, E. Zahid, D. K. Unruh, K. M. Hutchins , *IUCrJ*, 2022, **9**, 31-42.

MEVBIC/01/02/03/04/05: X. Ding, E. Zahid, D. K. Unruh, K. M. Hutchins , *IUCrJ*, 2022, **9**, 31-42.

MEVMIN/01/02/03/04/05: X. Ding, E. Zahid, D. K. Unruh, K. M. Hutchins , *IUCrJ*, 2022, **9**, 31-42.

MEVHUU/01/02/03/04/05: X. Ding, E. Zahid, D. K. Unruh, K. M. Hutchins , *IUCrJ*, 2022, **9**, 31-42.

MEVHUU06/07/08/09/10/11/12: X. Ding, D. K. Unruh, L. Ma, E. J. van Aalst, E. W. Reinheimer, B. J. Wylie and K. M. Hutchins, *Angew. Chem. Int. Ed.* 2023, **62**, e202306198.

LUJSEP: R. Kabe, H. Nakanotani, T. Sakanoue, M. Yahiro, C. Adachi, *Adv. Mater*., 2009, **21**, 4034-4038.

YAGSEG: H. Li, Y. Xiang, H. Han, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2011, **67**, o2953.

YAGSEG01: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

WILSOZ: W. Thyen, P. Zugenmaier, *Cryst. Res. Technol.,* 1994, **29**, 449-456.

WILSOZ01: P. Zugenmaier, *Int. J. Mol. Sci.*, 2011, **12**, 7360-7400.

WILSOZ02: Z. Fang, C. Cao, J. Chen, X. Deng, *J. Mol. Struct.*, 2014, **1063**, 307-312.

PYVINB: H. Nakanishi, W. Jones, G. M. Parkinson, *Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1979, **35**, 3103-3106.

PYVYBZ: H. Nakanishi, K. Ueno, M. Hasegawa, Y. Sasada, *Chem. Lett.,* 1972, **1**, 301-304.

HUJLED: N. Chanda, B. Mondal, V. G. Puranik, G. K. Lahiri, *Polyhedron*, 2002, **21**, 2033-2043.

HUJLED01: P. J. Ball, T. R. Shtoyko, J. A. K. Bauer, W. J. Oldham, W. B. Connick, *Inorg. Chem*., 2004, **43**, 622-632.

PUGBUP: L.-H. Huo, S. Gao, S. W. Ng, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2009, **65**, o2659.

LICGUC: N.-Y. Li, D. Liu, B. F. Abrahams, J.-P. Lang, *Chem. Commun*., 2018, **54**, 5831-5834.

ACICAR: H. N. Kim, H. K. Lee, S. W. Lee, *Bull. Korean Chem. Soc.*, 2005, **26**, 892-898.

ACICAR01: K. Ha, *Acta Crystallogr., Sect. E: Struct. Rep. Online*, 2011, **67**, o2250.

RUQTAZ: V. Stilinovic, D. Cincic, B. Kaitner, *Acta Chim. Slov.*, 2008, **55**, 874.

Table S5

KABKAB: G. Narayan, N. P. Rath, S. Das, *Acta Crystallogr., Sect. E: Struct. Rep. Online,* 2010, **66**, o2678.

ANISAZ: J.-L. Galigne, J. Falgueirettes, *Acta Crystallogr.,Sect. B: Struct. Crystallogr. Cryst. Chem.*, 1968, **24**, 1523-1529.

ANISAZ01: H. Astheimer, L. Walz, W. Haase, J. Loub, H. J. Muller, M. Gallardo, *Mol. Cryst. Liq. Cryst.,* 1985, **131**, 343-351.

ANISAZ02: S. V. Sereda, M. Yu. Antipin, T. V. Timofeeva, Yu.T. Struchkov, *Kristallografiya*, 1988, **33**, 118

ANISAZ03: S. Lakshmi, M. A. Sridhar, J. Shashidhara Prasad, J. Indira, P. P. Karat, B. Veerendra, B. Shivarama Holla, *Mol. Cryst. Liq. Cryst.*, 2002, **381**, 59-68.

ANISAZ04: B. Narayana, H. S. Yathirajan, B. K. Sarojini, M. Bolte, *CSD Communication*, 2007.

ANISAZ05: J.-Y. Jin, K. Zhang, L.-X. Zhang, A.-J. Zhang, Y.-Z. Liu, *Z. Kristallogr. - New Cryst. Struct.*, 2007, **222**, 391-392.

ANISAZ06: J. T. Mague, S. K. Mohamed, *CSD Communication*, 2016.

ANISAZ07: B. F. Abdel-Wahab, M. H. Alotaibi, G. A. El-Hiti, *CSD Communication*, 2017.

ANISAZ09: L. R. Gomes, J. N. Low, N. R. de L. Correira, T. C. M. Noguiera, A. C. Pinheiro, M. V. N. de Souza, J. L. Wardell, S. M. S. V. Wardell, *Z. Kristallogr. – Cryst. Mat.*, 2019, **234**, 59-71.

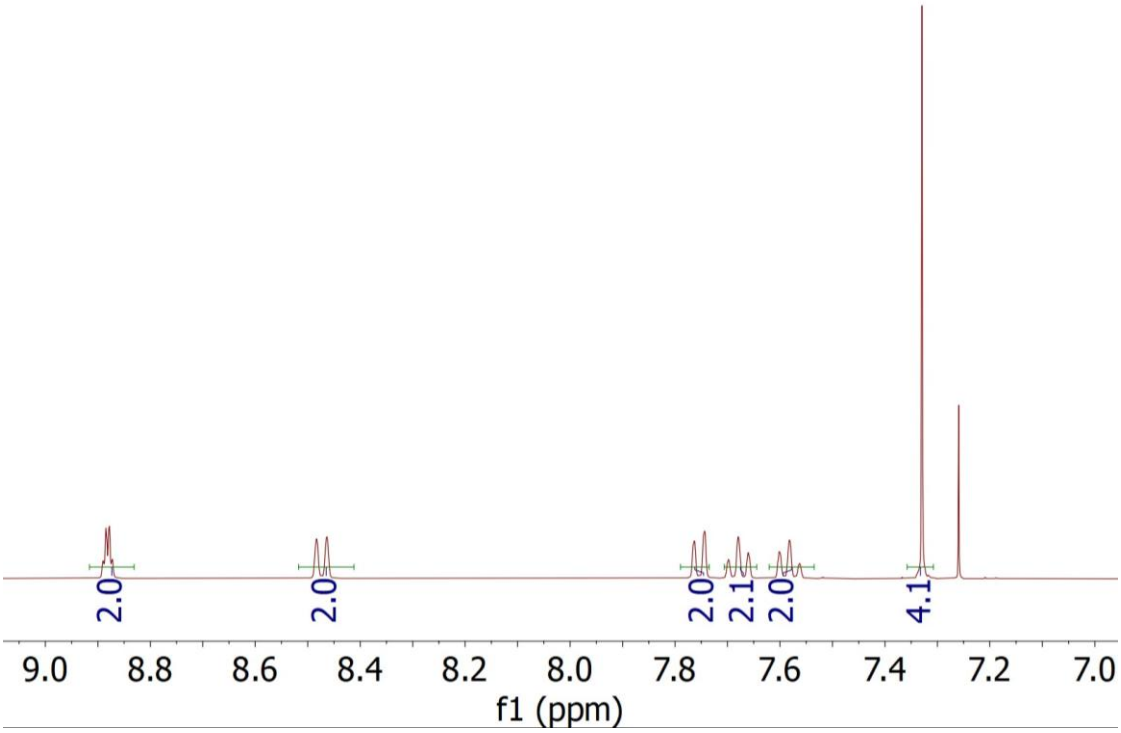
DIRJUN: E. Higgins, A. C. O'Donoghue, D. S. Yufit, J. A. K. Howard, *CSD Communication*, 2023.

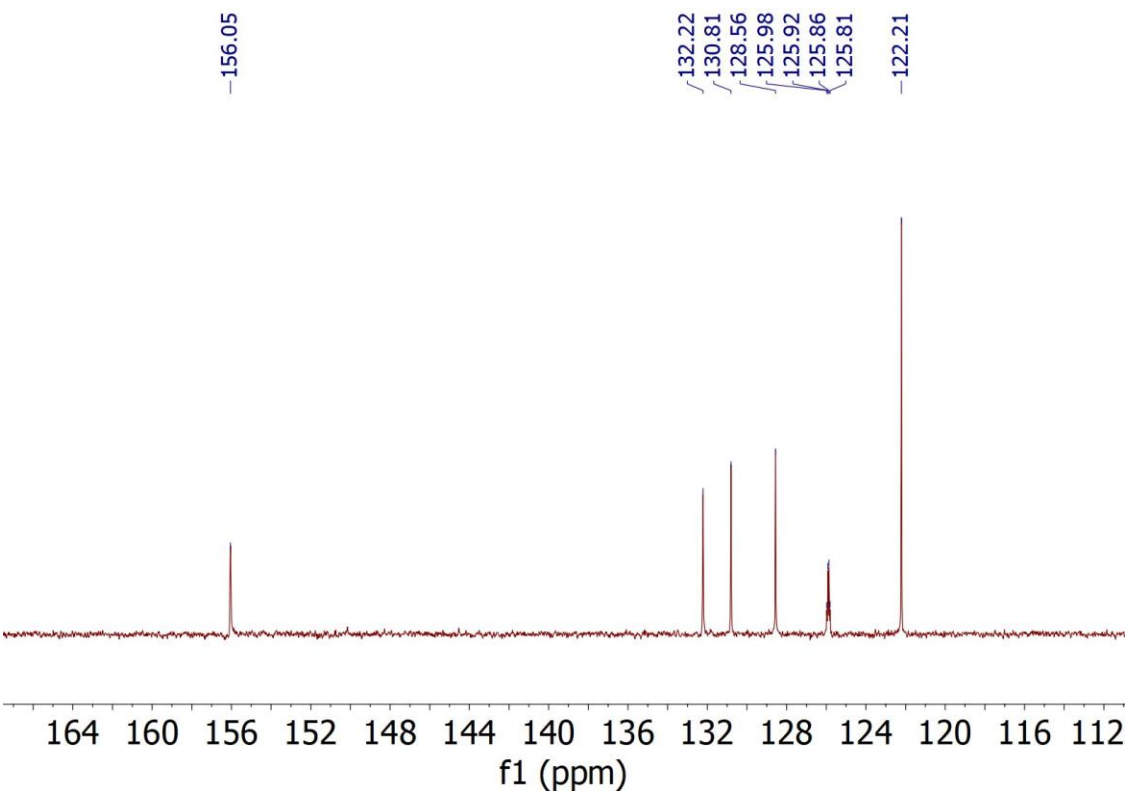
Table S6

WEFBOZ: Y. Yao, W. Shen, B. Nohra, C. Lescop, *Chem. Eur. J.,* 2010, **16**, 7143-7163; B. Nohra, S. Graule, C. Lescop, R. Reau, *J. Am. Chem. Soc*., 2006, **128**, 3520-3521.

HEWHEY: Z. Fang, C. Cao, *J. Mol. Struct.*, 2013, **1036**, 447-451.

DEWFIX: Z. Fang, F. Wu, Y. Jiao, N. Wang, C. Au, C. Cao, B. Yi, *J. Mol. Struct.,* 2018, **1159**, 147-155.





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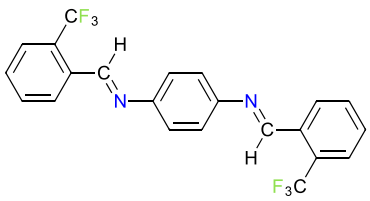
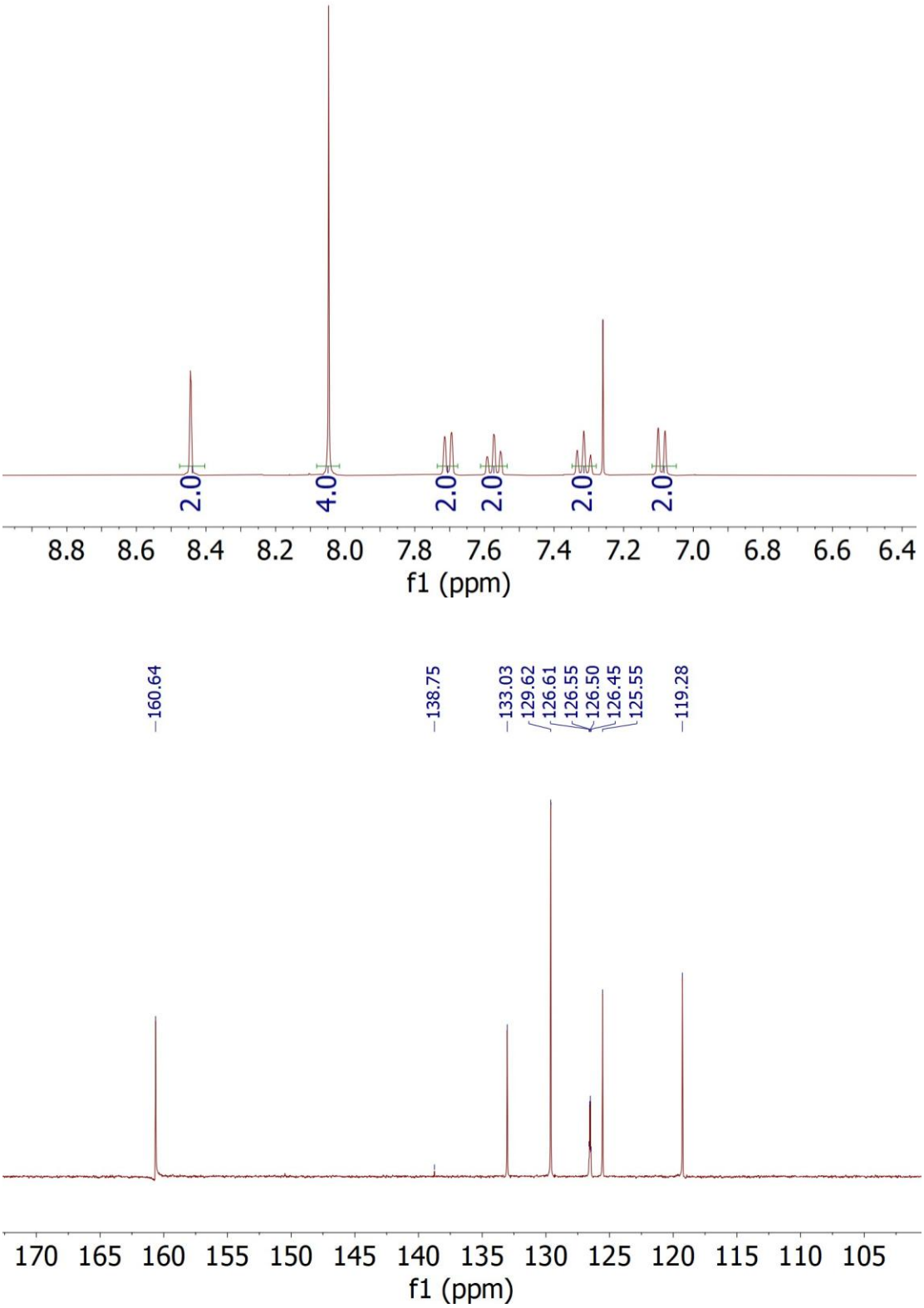
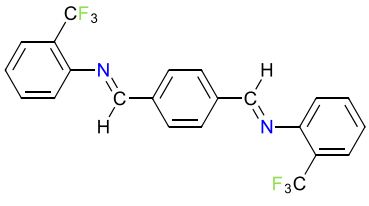
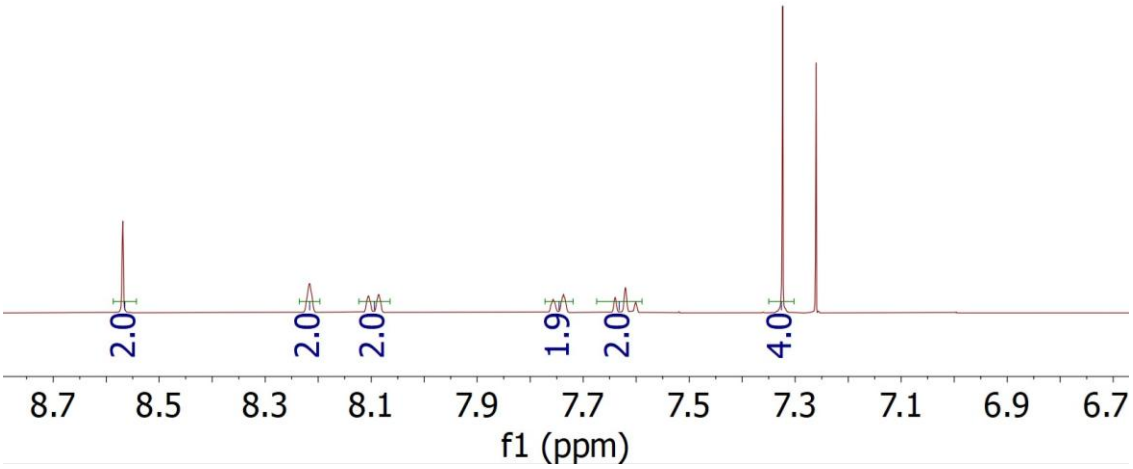
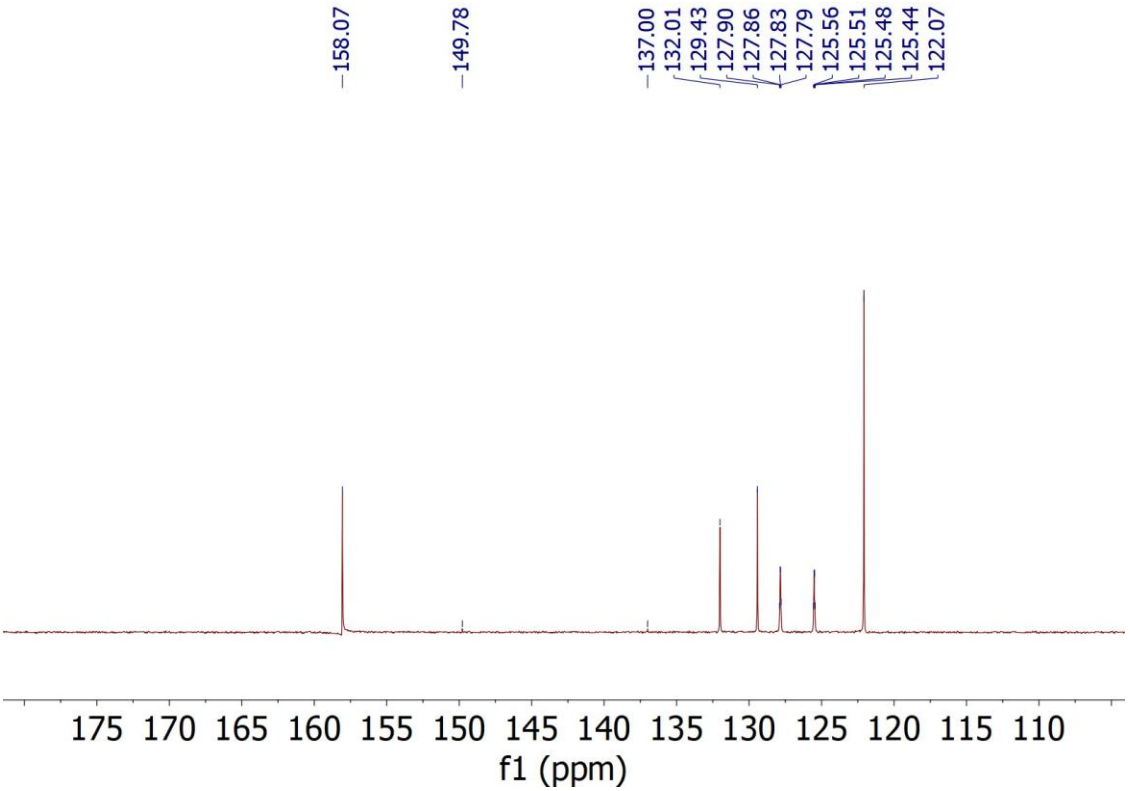




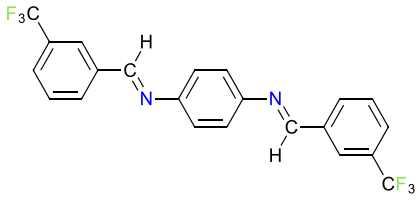
^{1}H-NMR (upper) and ^{13}C-NMR (lower) of **2-CC**

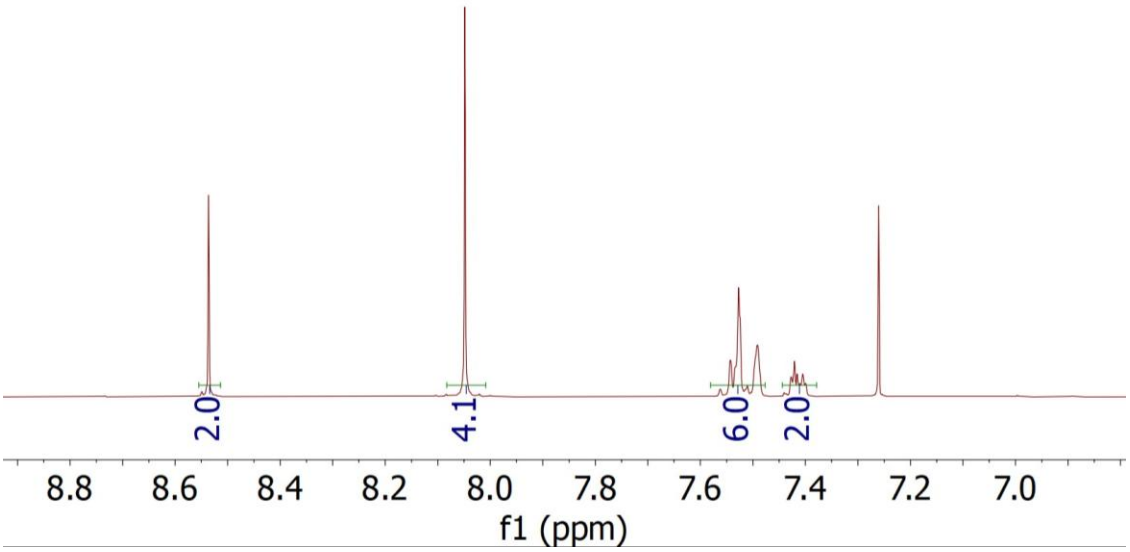


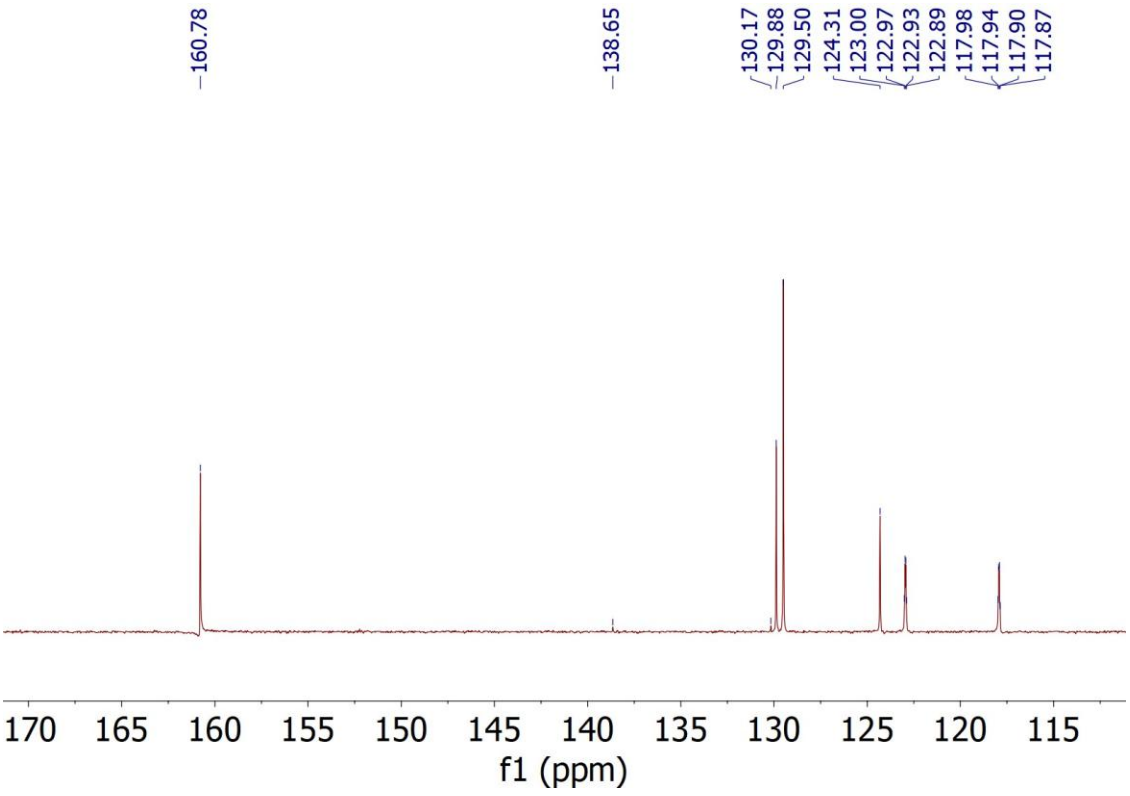




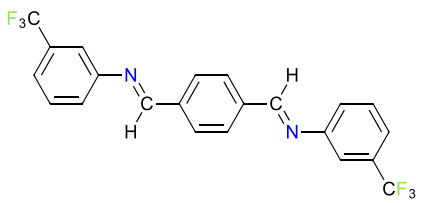
^{1}H-NMR (upper) and ^{13}C-NMR (lower) of **3-NN**

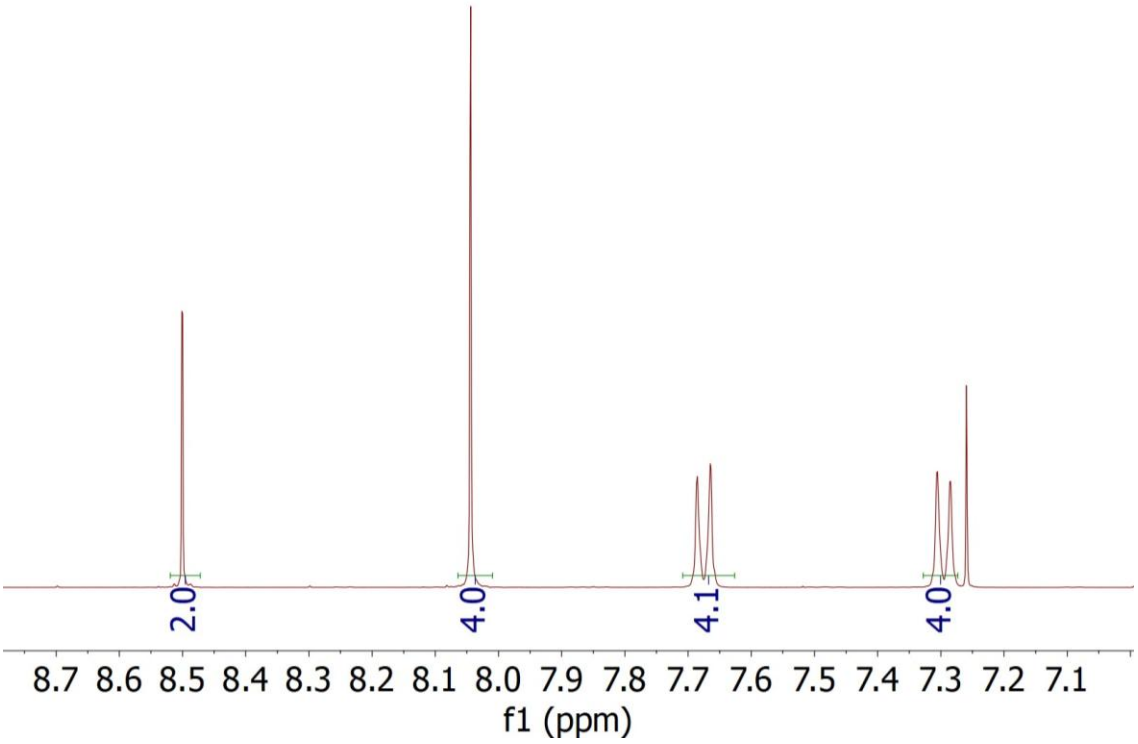


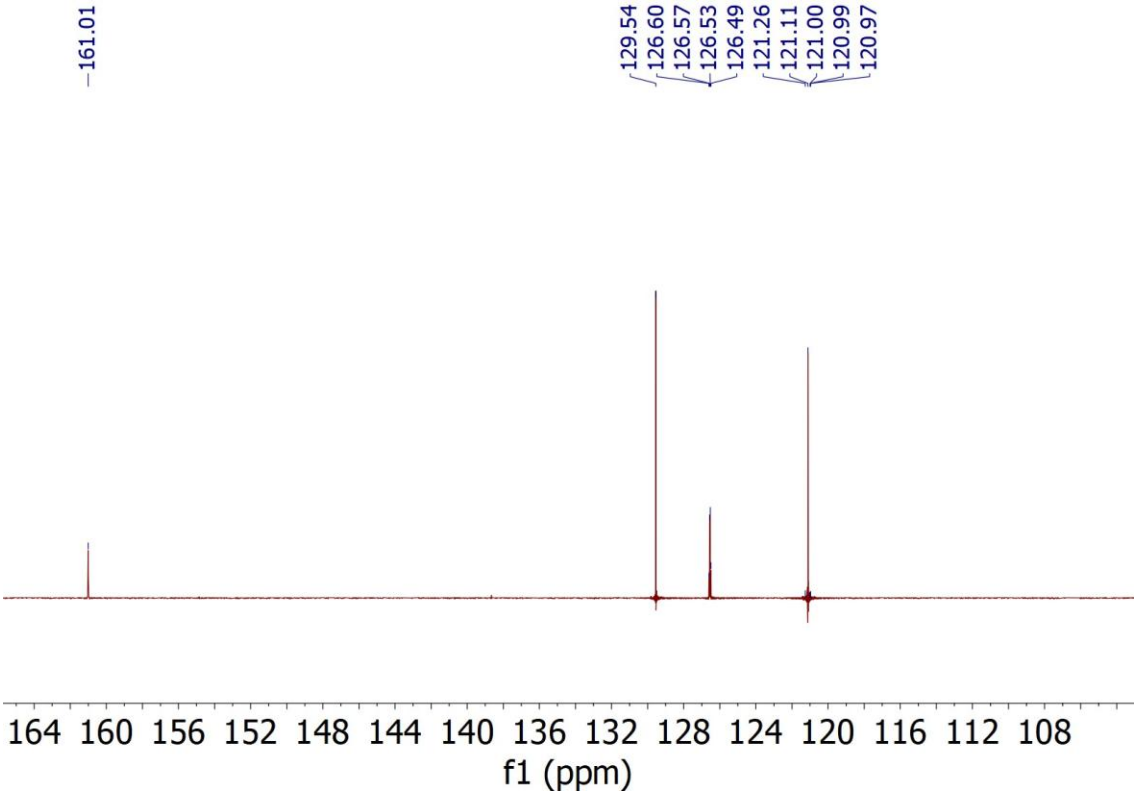




^{1}H-NMR (upper) and ^{13}C-NMR (lower) of **3-CC**







^{1}H-NMR (upper) and ^{13}C-NMR (lower) of **4-CC**