Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting information

Polymorphism in a 18-Membered Macrocycle: An Energetic and Topological Approach to Understand the Supramolecular Structure

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Summary

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Table S1. The normalized contact surface ($NC_{M1\cdots Mn}$)[a] and the normalized interaction energy ($NG_{M1\cdots Mn}$)[b] for dimers of the molecular cluster of compounds **1**,**2**, and **3**.

	1		**2**		**3**	
Dimer	$NC_{M1\cdots Mn}$	$NG_{M1\cdots Mn}$	$NC_{M1\cdots Mn}$	$NG_{M1\cdots Mn}$	$NC_{M1\cdots Mn}$	$NG_{M1\cdots Mn}$
M1...M2	3.43	4.51	2.70	3.36	3.43	3.85
M1...M3	3.43	4.51	2.70	3.36	3.43	3.85
M1...M4	0.72	1.01	1.02	0.81	1.04	0.38
M1...M5	0.51	0.17	1.10	0.94	1.27	1.13
M1...M6	0.72	1.01	1.02	0.81	1.27	1.13
M1...M7	0.51	0.17	1.10	0.94	1.04	0.38
M1...M8	0.42	0.42	1.10	0.94	0.59	0.73
M1...M9	1.10	0.80	1.02	0.81	0.59	0.73
M1...M10	0.65	0.44	1.10	0.94	1.08	0.94
M1...M11	0.42	0.42	1.02	0.81	1.08	0.94
M1...M12	1.10	0.80	0.04	0.07	0.59	0.73
M1...M13	0.65	0.44	0.04	0.07	0.59	0.73
M1...M14	0.42	0.42	0.04	0.07	1.08	0.94
M1...M15	1.10	0.80	0.04	0.07	1.08	0.94
M1...M16	0.65	0.44				
M1...M17	0.42	0.42				
M1...M18	1.10	0.80				
M1...M19	0.65	0.44				

[a]Determined using the equation $NC_{M1\cdots Mn} = MCN \times \frac{C_{M1\cdots Mn}}{C_{cluster}}$.[b]Determined using the equation $NG_{M1\cdots Mn} = MCN \times \frac{G_{M1\cdots Mn}}{G_{cluster}}$

Table S2. The ρ_{int} (from QTAIM)[a] and atom interaction energy (GAI)[b] for all dimers of compounds **1–3**.

1			**2**			**3**		
Interaction	ρ_{INT} (a.u.)	GAI(X···Y)b	Interaction	ρINT (a.u.)	GAI(X···Y)b	Interaction	ρINT (a.u.)	GAI(X···Y)b
Dimers M1···	M2, M3		Dimers M1···	M2, M3		Dimers M1···	M2, M3	
Acπ···πAc	0.003069	-1.56	CH···πPh	0.002189	-1.38	CH···πN	0.000894	-0.64
Phπ···πN	0.005833	-5.92		0.002189			0.000894	
	0.005833		Phπ···πAc	0.002864	-1.82	CH···πN	0.002192	-1.58
Acπ···πN	0.005990	-6.08		0.002864			0.002192	
	0.005990		Phπ···πAc	0.002929	-1.86	NH···πPh	0.003098	-2.24
Phπ···πN	0.006049	-6.14		0.002929			0.003098	
	0.006049		Phπ···πN	0.004838	-3.06	Phπ···πAc	0.004124	-2.98
Phπ···πPh	0.006080	-6.16		0.004838			0.004124	
	0.006080		Phπ···πN	0.005484	-3.48	Phπ···πAc	0.004316	-3.12
				0.005484			0.004316	
			Phπ···πN	0.005616	-3.56	Phπ···πN	0.005122	-3.72
				0.005616			0.005122	
			Phπ···πN	0.005769	-3.66	Phπ···πN	0.005220	-3.78
				0.005769			0.005220	
			Acπ···πN	0.006404	-4.06	Phπ···πPh	0.005408	-3.92
				0.006404			0.005408	
Dimers M1···	M4, M6		Dimers M1···	M4, M6, M9, M11		Dimers M1···	M4, M7	
Phπ···πPh	0.004213	-5.78	CH···πPh	0.001133	-0.36	CH···HC	0.000124	-0.02
	0.004213		CH···HC	0.002274	-0.72	CH···HC	0.002242	-0.66
			CH···πPh	0.002989	-0.95		0.002242	
			CH···πPh	0.003485	-1.10	CH···HC	0.002323	-0.68
			CH···πAc	0.007497	-2.38		0.002323	
						CH···HC	0.002703	-0.80
							0.002703	
Dimers M1···	M5, M7		Dimers M1···	M5, M7, M8, M10		Dimers M1···	M5, M6	
CH···HC	0.003570	-0.58	CH···πPh	0.003554	-3.02	CH···πPh	0.002624	-2.18
	0.003570			0.004235			0.002624	
CH···HC	0.004652	-0.38	CH···πPh	0.004355	-3.42	CH···πAc	0.002952	-2.46
				0.004460			0.002952	
						CH···HC	0.004341	-1.81
Dimers M1···	M8, M11, M14, M17		Dimers M1···	M12, M13, M14, M15		Dimers M1···	M8, M9, M12, M13	
CH···πPh	0.000003	-0.002	CH···HC	0.000034	-0.17	Phπ···πPh	0.002905	-1.32
CH···πPh	0.004907	-2.38	CH···πPh	0.000059	-0.29	CH···πPh	0.002984	-2.88
							0.003341	
Dimers M1···	M9, M12, M15, M18					Dimers M1···	M10, M11, M14, M15	
CH···πAc	0.002933	-1.12				CH···πPh	0.003061	-3.36
CH···πPh	0.004228	-1.61					0.003549	
CH···πPh	0.004851	-1.85				CH···HC	0.003954	-2.01
Dimers M1···	M10, M13, M16, M19							
CH···πPh	0.002095	-0.69						
CH···πAc	0.002643	-0.87						
CH···HC	0.002925	-0.96						

[a] Quantum Theory of Atoms in Molecules; [b] Interaction Energy (GAI(X···Y)[b]) in Kcal·Mol^{-1}, where X = CH, NH, π and Y = CH, π

Table S3. QTAIM data of dimers of polymorph **1**.

Dimer	Inter.[a]	ρ_{INT}	∇2ρ	Ellipticity	K	G_{AI}[b]
M1···M2	C···C	0.003069	+0.007735	2.043918	-0.000265	-1.56
	C···N	0.005833	+0.016198	0.151408	-0.000633	-2.96
	C···N	0.005833	+0.016198	0.151408	-0.000633	-2.96
	N···C	0.005990	+0.017332	0.762718	-0.000525	-3.04
M1···M3	C···N	0.005990	+0.017332	0.762719	-0.000525	-3.04
	C···N	0.006049	+0.016561	0.760642	-0.000447	-3.07
	N···C	0.006049	+0.016561	0.760641	-0.000447	-3.07
	C···C	0.006080	+0.015951	5.437158	-0.000605	-3.08
	C···C	0.006080	+0.015951	5.437147	-0.000605	-3.08
M1···M4 M1···M6	C···C	0.004213	+0.010093	4.547117	-0.000332	-2.89
	C···C	0.004213	+0.010093	4.547117	-0.000332	-2.89
M1···M5 M1···M7	H···H	0.003570	+0.015791	0.540647	-0.000987	-0.29
	H···H	0.003570	+0.015791	0.540647	-0.000987	-0.29
	H···H	0.004652	+0.019767	0.365183	-0.001185	-0.38
M1···M8 M1···M11 M1···M14 M1···M17	C-H···C	0.000003	+0.000026	0.832182	-0.000003	-0.002
	C-H···C	0.004907	+0.013273	0.831977	-0.000528	-2.38
M1···M9	C-H···C	0.002933	+0.009418	1.160748	-0.000510	-1.12
M1···M12 M1···M15 M1···M18	C-H···C	0.004228	+0.013612	0.548424	-0.000665	-1.61
	C-H···C	0.004851	+0.018013	2.579646	-0.001086	-1.85
M1···M10	C-H···C	0.002095	+0.006210	0.649268	-0.000351	-0.69
M1···M13 M1···M16 M1···M19	C-H···C	0.002643	+0.008068	0.368242	-0.000432	-0.87
	H···H	0.002925	+0.012743	0.374562	-0.000900	-0.96

[a] Atom···Atom interaction. [b] G_{AI} = Atom···Atom interaction energy kcal mol^{-1}

Table S4. QTAIM data of dimers of polymorp **2**.

Dimer	Inter.[a]	ρ_{INT}	∇2ρ	Ellipticity	K	G_{AI}[b]
M1···M2	C-H···C	0.002189	+0.006812	1.232112	-0.000430	-0.69
	C-H···C	0.002189	+0.006812	1.232112	-0.000430	-0.69
	C···C	0.002864	+0.007399	1.396501	-0.000306	-0.91
	C···C	0.002864	+0.007399	1.396501	-0.000306	-0.91
	C···C	0.002929	+0.006853	1.833869	-0.000257	-0.93
	C···C	0.002929	+0.006853	1.833869	-0.000257	-0.93
	C···N	0.004838	+0.013414	0.981098	-0.000501	-1.53
	C···N	0.004838	+0.013414	0.981098	-0.000501	-1.53
M1···M3	C···N	0.005484	+0.016050	3.137582	-0.000589	-1.74
	N···C	0.005484	+0.016050	3.137582	-0.000589	-1.74
	N···C	0.005616	+0.015589	0.891595	-0.000577	-1.78
	C···N	0.005616	+0.015589	0.891595	-0.000577	-1.78
	N···C	0.005769	+0.016022	2.073876	-0.000492	-1.83
	C···N	0.005769	+0.016022	2.073876	-0.000492	-1.83
	N···C	0.006404	+0.020497	0.612285	-0.000874	-2.03
	C···N	0.006404	+0.020497	0.612285	-0.000874	-2.03
M1···M4 M1···M6 M1···M9 M1···M11	C-H···C	0.001133	+0.004010	1.762601	-0.000273	-0.36
	H···H	0.002274	+0.009584	0.729230	-0.000731	-0.72
	C-H···C	0.002989	+0.009274	0.846358	-0.000511	-0.95
	C-H···C	0.003485	+0.011026	0.537803	-0.000599	-1.10
	C-H···C	0.007497	+0.023271	0.252554	-0.001043	-2.38
M1···M5 M1···M7 M1···M8 M1···M10	C-H···C	0.003554	+0.010928	0.382451	-0.000576	-1.38
	C-H···C	0.004235	+0.012663	0.493778	-0.000614	-1.64
	C-H···C	0.004355	+0.012686	0.534331	-0.000580	-1.69
	C-H···C	0.004460	+0.012953	1.079123	-0.000515	-1.73
M1···M12 M1···M13 M1···M14 M1···M15	H···H	0.000034	+0.000150	2.179692	-0.000012	-0.17
	C-H···C	0.000059	+0.000253	0.012823	-0.000023	-0.29

[a] Atom···Atom interaction. [b] G_{AI} = Atom···Atom interaction energy kcal mol^{-1}

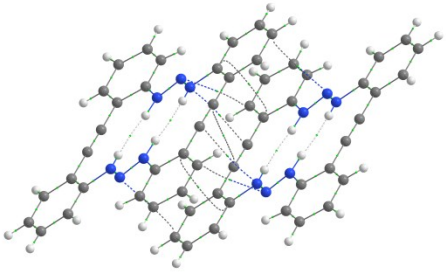
Table S5. QTAIM data of dimers of polymorph **3**.

Dimer	Inter.[a]	ρ_{INT}	∇2ρ	Ellipticity	K	G_{AI}[b]
M1···M2	C···N	0.000894	+0.003620	1.135797	-0.000260	-0.32
	C···N	0.000894	+0.003620	1.135797	-0.000260	-0.32
	C-H···N	0.002192	+0.008472	1.163303	-0.000590	-0.79
	N···H	0.002192	+0.008472	1.163303	-0.000590	-0.79
	N-H···C	0.003098	+0.011274	2.345392	-0.000576	-1.12
	C···H	0.003098	+0.011274	2.345392	-0.000576	-1.12
	C···C	0.004124	+0.010530	0.717869	-0.000490	-1.49
	C···C	0.004124	+0.010530	0.717869	-0.000490	-1.49
M1···M3	C···C	0.004316	+0.011809	0.664713	-0.000586	-1.56
	C···C	0.004316	+0.011809	0.664713	-0.000586	-1.56
	C···N	0.005122	+0.015260	7.829153	-0.000440	-1.86
	N···C	0.005122	+0.015260	7.829153	-0.000440	-1.86
	N···C	0.005220	+0.016455	0.649047	-0.000619	-1.89
	C···N	0.005220	+0.016455	0.649047	-0.000619	-1.89
	C···C	0.005408	+0.014837	1.577447	-0.000618	-1.96
	C···C	0.005408	+0.014837	1.577447	-0.000618	-1.96
M1···M4	H···H	0.000124	+0.000370	61.447185	-0.000029	-0.02
	H···H	0.002242	+0.010175	0.428670	-0.000725	-0.33
	H···H	0.002242	+0.010175	0.428670	-0.000725	-0.33
M1···M7	H···H	0.002323	+0.010879	0.966709	-0.000805	-0.34
	H···H	0.002323	+0.010879	0.966709	-0.000805	-0.34
	H···H	0.002703	+0.011886	0.221462	-0.000787	-0.40
	H···H	0.002703	+0.011886	0.221462	-0.000787	-0.40
M1···M5	C-H···C	0.002624	+0.009482	3.206180	-0.000678	-1.09
	C-H···C	0.002624	+0.009482	3.206180	-0.000678	-1.09
M1···M6	C-H···C	0.002952	+0.009262	2.246014	-0.000558	-1.23
	C-H···C	0.002952	+0.009262	2.246014	-0.000558	-1.23
	H···H	0.004341	+0.018131	9.975765	-0.001419	-1.81
M1···M8	C···C	0.002905	+0.008396	3.100721	-0.000427	-1.32
M1···M9	C-H···C	0.002984	+0.010120	1.231351	-0.000618	-1.36
M1···M12 M1···M13	C-H···C	0.003341	+0.010774	2.410194	-0.000489	-1.52
M1···M10	C-H··C	0.003061	+0.009939	1.541314	-0.000496	-1.56
M1···M11	CH···C	0.003549	+0.012442	0.420906	-0.000725	-1.80
M1···M14 M1···M15	H···H	0.003954	+0.016961	0.684578	-0.001155	-2.01

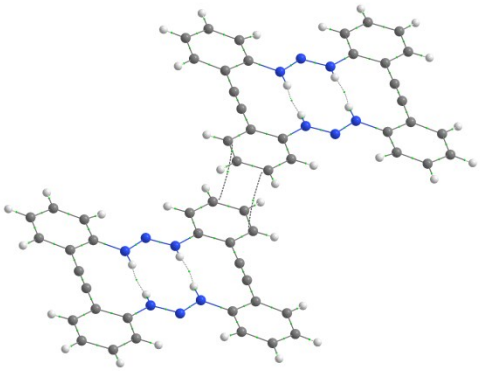
[a] Atom···Atom interaction. [b] G_{AI} = Atom···Atom interaction energy kcal mol^{-1}

Table S6. Symmetry codes of MN molecules of the molecular clusters of polymorphs **1**, **2** and **3**.

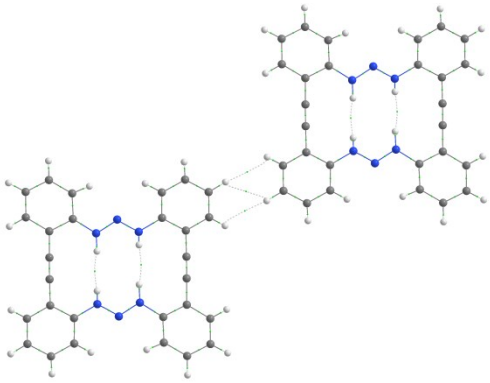
Dimer	Symmetry Code Polymorph **1**	Symmetry Code Polymorph **2**	Symmetry Code Polymorph **3**
M1	x,y,z	x,y,z	x,y,z
M2	1+x,y,z	x,y,1+z	x,1+y,z
M3	-1+x,y,z	x,y,-1+z	x,-1+y,z
M4	-x,1-y,-z	1/3+x-y,-1/3+x,2/3-z	-1+x,-1+y,z
M5	-1-x,1-y,-z	1/3+x-y,-1/3+x,-1/3+z	-1+x,y,z
M6	1+x,1+y,z	1/3+y,2/3-x+y,2/3-z	1+x,y,z
M7	2+x,1+y,z	1/3-y,-1/3+x-y,2/3+z	1+x,1+y,z
M8	1/2-x,1/2+y,1/2-z	2/3-x+y,1/3-x,-2/3+z	-1/2+x,1.5-y,-1/2+z
M9	1.5-x,1/2+y,1/2-z	2/3-x+y,1/3-x,1/3+z	-1/2+x,2.5-y,-1/2+z
M10	2.5-x,1/2+y,1/2-z	2/3-y,-2/3+x-y,-2/3+z	1/2+x,1.5-y,-1/2+z
M11	1/2-x,-1/2+y,1/2-z	2/3-y,-2/3+x-y,1/3+z	1/2+x,2.5-y,-1/2+z
M12	1.5-x,-1/2+y,1/2-z	1-y,x-y,z	1.5-x,-1/2+y,1/2-z
M13	2.5-x,-1/2+y,1/2-z	1-x+y,1-x,z	1.5-x,1/2+y,1/2+z
M14	1/2+x,1.5-y,-1/2+z	y,-x+y,1-z	1/2-x,-1/2+y,1/2-z
M15	-1/2+x,1.5-y,-1/2+z	x-y,-1+x,1-z	1/2-x,1/2+y,1/2-z
M16	-1.5+x,1.5-y,-1/2+z	. . .	. . .
M17	1/2+x,2.5-y,-1/2+z	. . .	. . .
M18	-1/2+x,2.5-y,-1/2+z	. . .	. . .
M19	-1.5+x,2.5-y,-1/2+z	. . .	. . .



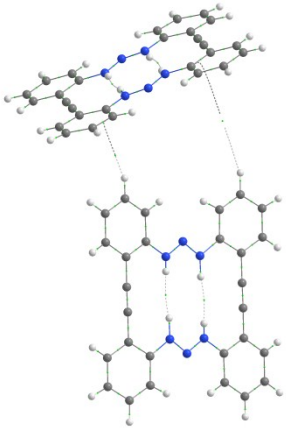
M1···M2 and M1···M3



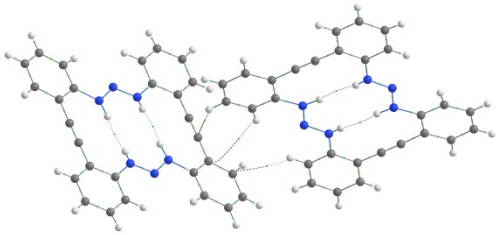
M1···M4 and M1···M6



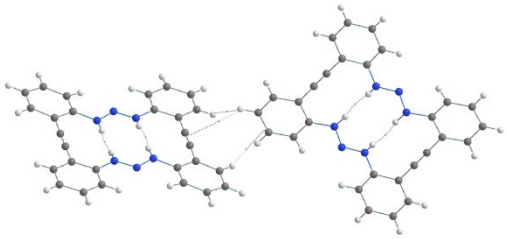
M1···M5 and M1···M7



M1···M8, M1···M11, M1···M14 and M1···M17

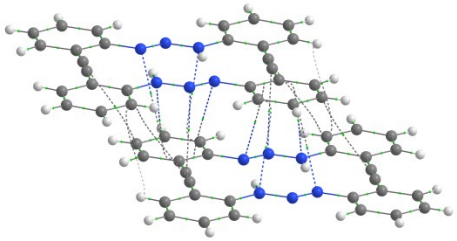


M1···M9, M1···M12, M1···M15 and M1···M18

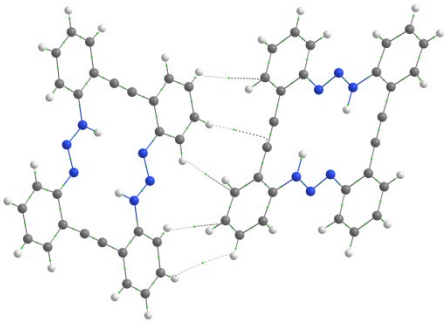


M1···M10, M1···M13, M1···M16 and M1···M19

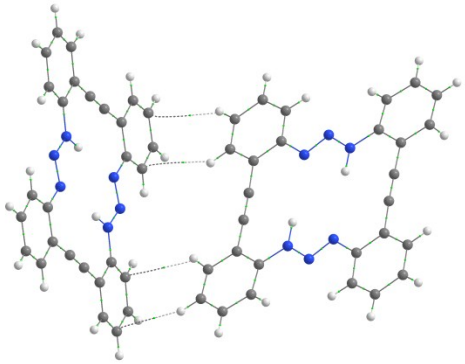
Fig. S1 View of BCPs connecting interacting atoms in polymorph **1**



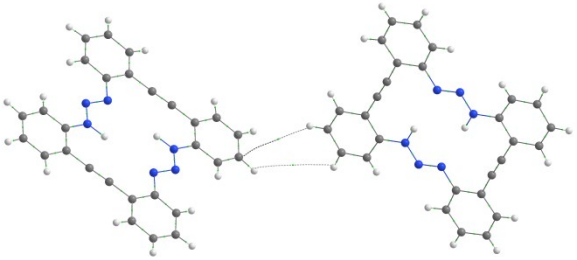
M1···M2 and M1···M3



M1···M4, M1···M6, M1···M9 and M1···M11

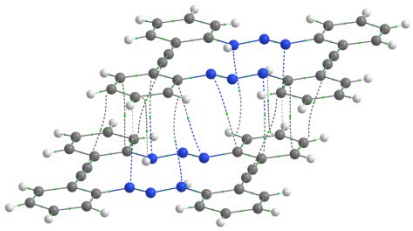


M1···M5, M1···M7, M1···M8 and M1···M10

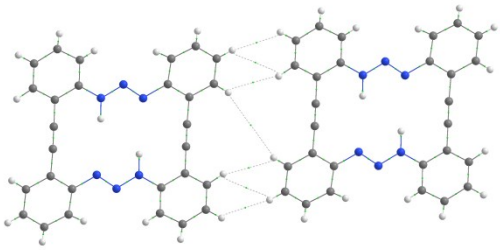


M1···M12, M1···M113, M1···M14 and M1···M15

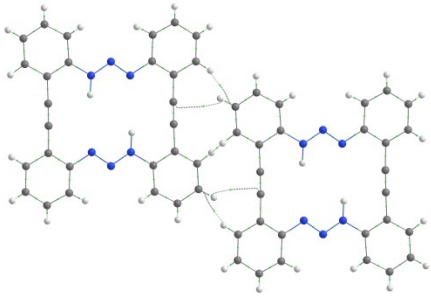
Fig. S2 View of BCPs connecting interacting atoms in polymorph **2**



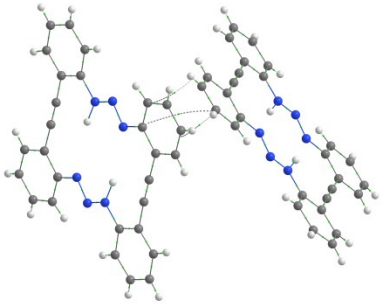
M1···M2 and M1···M3



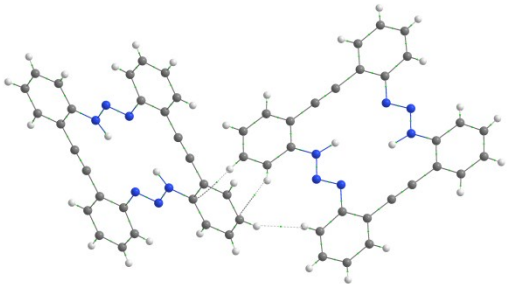
M1···M4 and M1···M7



M1···M5 and M1···M6



M1···M8, M1···M9, M1···M12 and M1···M13



M1···M10, M1···M11, M1···M14 and M1···M15

Fig. S3 View of BCPs connecting interacting atoms in polymorph **3**.