

Supporting information

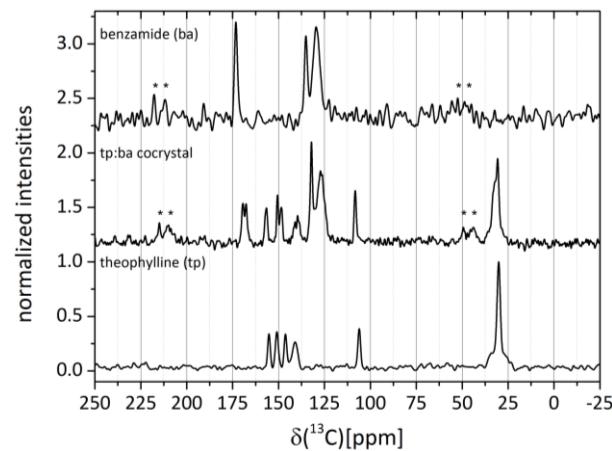


Figure S1 ^{13}C CPMAS NMR spectra of the tp:ba cocrystal and the reactants with the spinning sidebands(*).

S1. Computational details

Data Evaluation: DIFFRAC.SUITE EVA 4.0; structure solution DASH 3.3(David *et al.*, 2006); structure refinement: TOPAS(Coelho, 2007).

S2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters of experimental crystal structure from powder data.

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.14980(42)	0.04050(32)	0.83153(17)	0.04569
C2	0.28669(44)	0.09503(48)	0.83190(17)	0.04569
C3	0.08236(40)	0.01626(31)	0.78716(16)	0.04569
C4	0.08720(38)	0.01251(29)	0.87810(16)	0.04569
O5	0.35620(68)	0.09281(79)	0.87140(24)	0.04569
N6	0.33672(47)	0.14009(53)	0.78775(16)	0.04569
C7	-0.04437(39)	-0.03459(30)	0.78751(16)	0.04569
H8	0.1232(17)	0.0346(19)	0.75248(66)	0.05483
C9	-0.03679(39)	-0.03723(29)	0.87881(16)	0.04569
H10	0.1322(20)	0.0281(19)	0.91065(67)	0.05483
H11	0.4037(16)	0.2066(18)	0.79406(61)	0.05483
H12	0.3011(21)	0.1603(17)	0.75353(67)	0.05483
C13	-0.10385(36)	-0.06142(29)	0.83266(16)	0.04569
H14	-0.0885(17)	-0.0496(18)	0.75389(70)	0.05483
H15	-0.0799(18)	-0.0560(18)	0.91148(68)	0.05483
H16	-0.1916(17)	-0.0965(15)	0.83187(83)	0.05483

N17	0.77295(71)	0.66539(46)	0.64541(16)	0.04569
C18	0.81538(82)	0.56520(46)	0.61405(17)	0.04569
C19	0.79086(45)	0.64782(42)	0.70053(18)	0.04569
C20	0.72087(85)	0.78561(47)	0.63011(17)	0.04569
N21	0.79641(71)	0.57922(44)	0.56265(16)	0.04569
O22	0.85660(80)	0.46349(60)	0.63127(27)	0.04569
H23	0.8421(20)	0.5722(20)	0.70736(91)	0.05483
H24	0.8329(21)	0.7219(16)	0.71369(62)	0.05483
H25	0.7094(18)	0.6372(18)	0.71633(70)	0.05483
C26	0.70941(85)	0.78797(48)	0.57544(17)	0.04569
O27	0.68332(76)	0.86670(64)	0.65998(23)	0.04569
C28	0.75140(88)	0.69319(46)	0.54358(16)	0.04569
C29	0.84411(44)	0.47657(41)	0.52873(15)	0.04569
N30	0.66739(63)	0.88826(44)	0.54528(16)	0.04569
N31	0.73198(82)	0.72552(56)	0.49446(20)	0.04569
H32	0.8650(18)	0.3993(16)	0.54809(63)	0.05483
H33	0.9193(18)	0.5080(19)	0.51187(73)	0.05483
H34	0.7783(20)	0.4566(19)	0.50423(67)	0.05483
C35	0.68579(78)	0.84575(46)	0.49707(17)	0.04569
H36	0.6192(17)	0.9567(15)	0.55522(68)	0.05483
H37	0.6616(18)	0.9010(18)	0.46646(71)	0.05483
C38	0.46207(32)	0.65991(42)	0.11543(16)	0.04569
C39	0.40872(47)	0.79610(43)	0.11160(17)	0.04569
C40	0.48616(31)	0.60345(40)	0.16187(16)	0.04569
C41	0.48704(29)	0.59046(38)	0.07091(16)	0.04569
O42	0.40482(79)	0.85624(67)	0.06951(23)	0.04569
N43	0.37922(89)	0.85449(45)	0.15581(16)	0.04569
C44	0.53470(32)	0.47807(39)	0.16483(16)	0.04569
H45	0.4695(22)	0.6520(21)	0.19543(68)	0.05483
C46	0.53541(30)	0.46568(39)	0.07265(16)	0.04569
H47	0.4707(17)	0.6314(17)	0.03769(67)	0.05483
H48	0.3838(23)	0.9498(18)	0.15306(67)	0.05483
H49	0.3904(40)	0.8328(19)	0.19280(64)	0.05483
C50	0.55979(33)	0.40820(36)	0.12160(16)	0.04569
H51	0.5510(18)	0.4415(19)	0.19967(71)	0.05483
H52	0.5531(18)	0.4163(17)	0.04052(67)	0.05483
H53	0.5930(16)	0.3202(19)	0.12532(69)	0.05483
N54	0.17071(45)	0.72266(71)	0.28773(16)	0.04569
C55	0.06470(46)	0.69265(93)	0.31895(17)	0.04569
C56	0.15359(41)	0.69941(43)	0.23330(18)	0.04569
C57	0.29008(47)	0.77652(85)	0.30278(17)	0.04569
N58	0.08458(43)	0.69546(65)	0.37094(16)	0.04569
O59	-0.03712(60)	0.65096(92)	0.30091(26)	0.04569
H60	0.0681(18)	0.6635(18)	0.22668(78)	0.05483
H61	0.1626(20)	0.7789(16)	0.21600(64)	0.05483
H62	0.2181(19)	0.6392(17)	0.22241(60)	0.05483

C63	0.29106(47)	0.79255(82)	0.35765(17)	0.04569
O64	0.37339(62)	0.80111(74)	0.27251(25)	0.04569
C65	0.19370(47)	0.75321(79)	0.38978(16)	0.04569
C66	-0.02455(40)	0.65971(42)	0.40385(14)	0.04569
N67	0.38922(47)	0.83765(72)	0.38882(16)	0.04569
N68	0.22245(54)	0.77737(90)	0.43896(20)	0.04569
H69	-0.0970(16)	0.6329(17)	0.38393(69)	0.05483
H70	-0.0488(17)	0.7318(21)	0.42394(66)	0.05483
H71	0.0026(20)	0.5886(17)	0.42481(65)	0.05483
C72	0.34394(46)	0.82392(74)	0.43681(17)	0.04569
H73	0.4590(15)	0.8864(19)	0.37922(73)	0.05483
H74	0.3950(20)	0.8583(19)	0.46706(87)	0.05483

S3. Fractional atomic coordinates of DFT calculation data.

	x	y	z
O1	0.85281	0.45368	0.6284
O2	0.6874	0.86635	0.66206
N1	0.77626	0.66325	0.64397
N2	0.67334	0.89841	0.54331
N3	0.73714	0.73431	0.49099
N4	0.8026	0.58114	0.55866
C1	0.81297	0.55925	0.61125
C2	0.72225	0.78425	0.62899
C3	0.7152	0.7973	0.57457
C4	0.68871	0.85651	0.49423
C5	0.75419	0.69825	0.54098
C6	0.8406	0.47542	0.52375
C7	0.79417	0.64125	0.69906
H1	0.78938	0.38521	0.53453
H2	0.94649	0.45787	0.52592
H3	0.81384	0.5035	0.48452
H4	0.66551	0.9157	0.46067
H5	0.64448	0.99196	0.55549
H6	0.87704	0.57544	0.70467
H7	0.81059	0.73529	0.71803
H8	0.70665	0.59585	0.7158
O3	-0.03437	0.63824	0.30109
O4	0.38217	0.80151	0.27209
N5	0.17571	0.71789	0.28779
N6	0.39713	0.83578	0.39074
N7	0.22854	0.7749	0.44078
N8	0.08528	0.69664	0.37193
C8	0.06866	0.6817	0.31918
C9	0.29468	0.77223	0.30418
C10	0.30101	0.78782	0.35841
C11	0.35022	0.82568	0.43906
C12	0.19846	0.75069	0.39062
C13	-0.02189	0.65749	0.40592
C14	0.16046	0.69928	0.23239
H9	-0.06415	0.56585	0.3918
H10	-0.09845	0.73258	0.40735
H11	0.01725	0.6428	0.44467
H12	0.40405	0.85586	0.47315
H13	0.49155	0.86798	0.38032
H14	0.06814	0.64939	0.22538
H15	0.16042	0.79407	0.21265
H16	0.24081	0.64036	0.21707
O5	0.35039	0.08927	0.87217

N9	0.33729	0.14767	0.78781
C15	0.28543	0.09775	0.8309
C16	0.14749	0.04759	0.82935
C17	0.07823	0.02701	0.78325
C18	-0.0484	-0.02445	0.78436
C19	-0.1081	-0.05544	0.83129
C20	-0.03955	-0.03478	0.87715
C21	0.0871	0.01554	0.87623
H17	0.43418	0.17432	0.78794
H18	0.28442	0.16718	0.75474
H19	0.14152	0.03033	0.91187
H20	-0.08553	-0.058	0.91389
H21	-0.20709	-0.09538	0.83247
H22	-0.10118	-0.04095	0.74834
H23	0.1227	0.05081	0.74624
O6	0.38862	0.84563	0.07131
N10	0.37634	0.86251	0.15853
C22	0.40302	0.79552	0.11533
C23	0.45449	0.65827	0.12016
C24	0.48669	0.60005	0.16755
C25	0.53906	0.47394	0.1691
C26	0.56008	0.40393	0.12358
C27	0.52825	0.46101	0.07631
C28	0.47623	0.58711	0.07472
H24	0.34756	0.95907	0.15586
H25	0.38491	0.82408	0.19465
H26	0.4529	0.63392	0.03816
H27	0.54513	0.40697	0.04067
H28	0.6028	0.30624	0.12506
H29	0.56705	0.42964	0.20569
H30	0.47332	0.65295	0.2037

S4. Geometric parameters of crystal structure from powder data.

O22 - C18 1.215(9)	O27 - C20 1.207(8)	N17 - C18 1.387(7)	N17 - C19 1.465(6)
N17 - C20 1.405(8)	N21 - C18 1.366(6)	N21 - C28 1.355(7)	N21 - C29 1.463(6)
N30 - C26 1.368(7)	N30 - C35 1.348(6)	N31 - C28 1.341(7)	N31 - C35 1.327(9)
C20 - C26 1.435(6)	C26 - C28 1.353(8)		
N30 - H36 0.899(17)	C19 - H23 0.96(2)	C19 - H24 0.942(18)	C19 - H25 0.940(19)
C29 - H32 0.967(17)	C29 - H33 0.947(19)	C29 - H34 0.96(2)	C35 - H37 1.012(19)
O59 - C55 1.226(9)	O64 - C57 1.194(9)	N54 - C55 1.396(7)	N54 - C56 1.455(6)
N54 - C57 1.403(8)	N58 - C55 1.376(6)	N58 - C65 1.361(8)	N58 - C66 1.462(6)
N67 - C63 1.377(7)	N67 - C72 1.347(6)	N68 - C65 1.344(7)	N68 - C72 1.338(8)
C57 - C63 1.445(6)	C63 - C65 1.369(7)		
N67 - H73 0.911(18)	C56 - H60 0.969(19)	C56 - H61 0.939(17)	C56 - H62 0.951(19)

C66	-	H69	0.950(17)	C66	-	H70	0.94(2)	C66	-	H71	0.957(19)	C72	-	H74	1.01(2)
O5	-	C2	1.257(7)	N6	-	C2	1.347(6)	C1	-	C2	1.515(6)	C1	-	C3	1.375(6)
C1	-	C4	1.408(6)	C3	-	C7	1.405(6)	C4	-	C9	1.374(6)	C7	-	C13	1.358(6)
C9	-	C13	1.413(6)	--	--	--	--	--	--	--	--	--	--	--	--
N6	-	H11	0.985(18)	N6	-	H12	0.990(19)	C3	-	H8	1.017(19)	C4	-	H10	0.982(19)
C7	-	H14	1.001(19)	C9	-	H15	0.982(19)	C13	-	H16	0.971(18)	--	--	--	--
O42	-	C39	1.263(7)	N43	-	C39	1.338(6)	C38	-	C39	1.507(6)	C38	-	C40	1.369(6)
C38	-	C41	1.390(6)	C40	-	C44	1.385(6)	C41	-	C46	1.377(6)	C44	-	C50	1.365(6)
C46	-	C50	1.433(6)	--	--	--	--	--	--	--	--	--	--	--	--
N43	-	H48	0.984(19)	N43	-	H49	0.999(17)	C40	-	H45	1.023(19)	C41	-	H47	0.980(19)
C44	-	H51	1.001(19)	C46	-	H52	0.999(19)	C50	-	H53	0.97(2)				

C18	-	N17	-	C19	116.8(5)	C18	-	N17	-	C20	127.2(4)	C19	-	N17	-	C20	115.9(4)
C18	-	N21	-	C28	120.1(4)	C18	-	N21	-	C29	118.2(5)	C28	-	N21	-	C29	121.0(4)
C26	-	N30	-	C35	104.5(4)	C28	-	N31	-	C35	103.6(5)	O22	-	C18	-	N17	121.9(5)
O22	-	C18	-	N21	120.4(6)	N17	-	C18	-	N21	117.3(5)	O27	-	C20	-	N17	123.1(5)
O27	-	C20	-	C26	127.4(6)	N17	-	C20	-	C26	109.3(5)	N30	-	C26	-	C20	127.8(5)
N30	-	C26	-	C28	106.8(4)	C20	-	C26	-	C28	125.1(5)	N21	-	C28	-	N31	128.1(5)
N21	-	C28	-	C26	120.3(4)	N31	-	C28	-	C26	111.3(6)	N30	-	C35	-	N31	113.6(5)
C26	-	N30	-	H36	126.7(12)	C35	-	N30	-	H36	127.0(13)	N17	-	C19	-	H23	110.8(15)
N17	-	C19	-	H24	108.5(10)	N17	-	C19	-	H25	109.5(12)	H23	-	C19	-	H24	109.8(18)
H23	-	C19	-	H25	108.2(18)	H24	-	C19	-	H25	110.1(17)	N21	-	C29	-	H32	110.5(10)
N21	-	C29	-	H33	108.1(12)	N21	-	C29	-	H34	108.9(13)	H32	-	C29	-	H33	110.0(16)
H32	-	C29	-	H34	109.4(16)	H33	-	C29	-	H34	110.0(17)	N30	-	C35	-	H37	121.5(12)
N31	-	C35	-	H37	124.8(11)												
C55	-	N54	-	C56	116.2(4)	C55	-	N54	-	C57	127.3(4)	C56	-	N54	-	C57	116.5(4)
C55	-	N58	-	C65	119.3(5)	C55	-	N58	-	C66	117.6(4)	C65	-	N58	-	C66	122.0(4)
C63	-	N67	-	C72	105.3(5)	C65	-	N68	-	C72	103.3(5)	O59	-	C55	-	N54	121.2(5)
O59	-	C55	-	N58	121.0(6)	N54	-	C55	-	N58	117.2(5)	O64	-	C57	-	N54	121.7(5)
O64	-	C57	-	C63	129.0(6)	N54	-	C57	-	C63	109.3(4)	N67	-	C63	-	C57	129.2(5)
N67	-	C63	-	C65	105.8(4)	C57	-	C63	-	C65	124.8(5)	N58	-	C65	-	N68	127.5(5)
N58	-	C65	-	C63	120.6(4)	N68	-	C65	-	C63	111.9(5)	N67	-	C72	-	N68	113.6(5)
C63	-	N67	-	H73	126.8(12)	C72	-	N67	-	H73	126.0(13)	N54	-	C56	-	H60	110.3(13)
N54	-	C56	-	H61	108.4(11)	N54	-	C56	-	H62	108.5(11)	H60	-	C56	-	H61	109.8(17)
H60	-	C56	-	H62	109.4(16)	H61	-	C56	-	H62	110.5(16)	N58	-	C66	-	H69	110.6(11)
N58	-	C66	-	H70	109.4(12)	N58	-	C66	-	H71	107.6(13)	H69	-	C66	-	H70	109.1(16)
H69	-	C66	-	H71	109.0(16)	H70	-	C66	-	H71	111.2(16)	N67	-	C72	-	H74	120.8(13)
N68	-	C72	-	H74	125.1(13)												
C2	-	C1	-	C3	122.7(4)	C2	-	C1	-	C4	119.7(4)	C3	-	C1	-	C4	117.6(4)
O5	-	C2	-	N6	119.6(5)	O5	-	C2	-	C1	121.8(5)	N6	-	C2	-	C1	118.5(4)
C1	-	C3	-	C7	122.0(4)	C1	-	C4	-	C9	120.8(4)	C3	-	C7	-	C13	120.0(4)
C4	-	C9	-	C13	120.5(4)	C7	-	C13	-	C9	119.2(4)						
C2	-	N6	-	H11	111.2(10)	C2	-	N6	-	H12	135.0(13)	H11	-	N6	-	H12	105.4(15)
C1	-	C3	-	H8	120.8(11)	C7	-	C3	-	H8	117.2(11)	C1	-	C4	-	H10	120.2(12)
C9	-	C4	-	H10	119.0(12)	C3	-	C7	-	H14	118.2(11)	C13	-	C7	-	H14	121.9(11)
C4	-	C9	-	H15	120.2(12)	C13	-	C9	-	H15	119.3(11)	C7	-	C13	-	H16	118.4(13)

C9	-	C13	-	H16	122.4(13)												
C39	-	C38	-	C40	121.2(4)	C39	-	C38	-	C41	119.2(4)	C40	-	C38	-	C41	119.5(4)
O42	-	C39	-	N43	121.8(5)	O42	-	C39	-	C38	121.6(5)	N43	-	C39	-	C38	116.2(4)
C38	-	C40	-	C44	120.6(4)	C38	-	C41	-	C46	121.2(4)	C40	-	C44	-	C50	120.8(4)
C41	-	C46	-	C50	118.5(4)	C44	-	C50	-	C46	119.4(4)						
C39	-	N43	-	H48	111.9(12)	C39	-	N43	-	H49	135.4(16)	H48	-	N43	-	H49	106.7(16)
C38	-	C40	-	H45	121.7(12)	C44	-	C40	-	H45	117.7(12)	C38	-	C41	-	H47	119.4(11)
C46	-	C41	-	H47	119.4(11)	C40	-	C44	-	H51	117.5(12)	C50	-	C44	-	H51	121.7(12)
C41	-	C46	-	H52	120.8(11)	C50	-	C46	-	H52	120.7(11)	C44	-	C50	-	H53	118.3(12)
C46	-	C50	-	H53	122.3(11)												

O22	C18	N17	C19	5.3(11)	O22	C18	N17	C20	-178.4(8)	N21	C18	N17	C19	178.5(6)
N21	C18	N17	C20	-5.3(12)	O22	C18	N21	C28	-179.5(8)	O22	C18	N21	C29	-8.6(11)
N17	C18	N21	C28	7.2(11)	N17	C18	N21	C29	178.1(6)	O27	C20	N17	C18	178.2(9)
O27	C20	N17	C19	-5.5(12)	C26	C20	N17	C18	3.7(12)	C26	C20	N17	C19	180.0(6)
O27	C20	C26	N30	8.2(15)	O27	C20	C26	C28	-178.8(9)	N17	C20	C26	N30	-177.6(8)
N17	C20	C26	C28	-4.6(12)	C20	C26	N30	C35	174.7(9)	C28	C26	N30	C35	0.7(9)
N30	C26	C28	N21	-178.5(7)	N30	C26	C28	N31	-3.2(10)	C20	C26	C28	N21	7.3(14)
C20	C26	C28	N31	-177.4(8)	N31	C28	N21	C18	177.2(9)	N31	C28	N21	C29	6.6(13)
C26	C28	N21	C18	-8.4(12)	C26	C28	N21	C29	-179.0(7)	N21	C28	N31	C35	179.1(9)
C26	C28	N31	C35	4.3(10)	N31	C35	N30	C26	2.0(9)	N30	C35	N31	C28	-3.9(10)
H23	C19	N17	C18	8.2(15)	H23	C19	N17	C20	-168.5(14)	H24	C19	N17	C18	128.7(14)
H24	C19	N17	C20	-48.0(15)	H25	C19	N17	C18	-111.1(14)	H25	C19	N17	C20	72.2(14)
C20	C26	N30	H36	-20.0(19)	C28	C26	N30	H36	166.1(15)	H32	C29	N21	C18	14.5(14)
H32	C29	N21	C28	-174.8(13)	H33	C29	N21	C18	-106.0(13)	H33	C29	N21	C28	64.8(14)
H34	C29	N21	C18	134.6(14)	H34	C29	N21	C28	-54.6(15)	N31	C35	N30	H36	-163.3(15)
H37	C35	N30	C26	179.2(14)	H37	C35	N30	H36	14(2)	H37	C35	N31	C28	179.0(15)
O59	C55	N54	C56	-1.1(12)	O59	C55	N54	C57	176.8(9)	N58	C55	N54	C56	170.6(6)
N58	C55	N54	C57	-11.5(13)	O59	C55	N58	C65	-174.1(8)	O59	C55	N58	C66	-6.2(12)
N54	C55	N58	C65	14.2(11)	N54	C55	N58	C66	-177.9(6)	O64	C57	N54	C55	-178.2(8)
O64	C57	N54	C56	-0.4(12)	C63	C57	N54	C55	2.5(12)	C63	C57	N54	C56	-179.7(6)
O64	C57	C63	N67	-1.5(16)	O64	C57	C63	C65	-175.3(9)	N54	C57	C63	N67	177.7(8)
N54	C57	C63	C65	4.0(11)	C57	C63	N67	C72	-175.4(8)	C65	C63	N67	C72	-0.7(8)
N67	C63	C65	N58	-175.9(7)	N67	C63	C65	N68	3.3(9)	C57	C63	C65	N58	-0.9(12)
C57	C63	C65	N68	178.3(8)	N68	C65	N58	C55	172.3(8)	N68	C65	N58	C66	4.9(12)
C63	C65	N58	C55	-8.7(11)	C63	C65	N58	C66	-176.1(6)	N58	C65	N68	C72	174.7(8)
C63	C65	N68	C72	-4.4(10)	N68	C72	N67	C63	-2.1(9)	N67	C72	N68	C65	4.0(10)
H60	C56	N54	C55	-1.1(14)	H60	C56	N54	C57	-179.2(13)	H61	C56	N54	C55	119.2(15)
H61	C56	N54	C57	-58.9(15)	H62	C56	N54	C55	-120.8(13)	H62	C56	N54	C57	61.1(14)
C57	C63	N67	H73	20(2)	C65	C63	N67	H73	-165.5(16)	H69	C66	N58	C55	3.6(14)
H69	C66	N58	C65	171.2(13)	H70	C66	N58	C55	-116.5(13)	H70	C66	N58	C65	51.1(14)
H71	C66	N58	C55	122.6(13)	H71	C66	N58	C65	-69.9(14)	N68	C72	N67	H73	162.9(16)
H74	C72	N67	C63	-174.2(15)	H74	C72	N67	H73	-9(2)	H74	C72	N68	C65	175.7(15)
C3	C1	C2	O5	-165.8(6)	C3	C1	C2	N6	10.5(6)	C4	C1	C2	O5	14.1(7)
C4	C1	C2	N6	-169.7(4)	C2	C1	C3	C7	179.8(3)	C4	C1	C3	C7	0.0(5)
C2	C1	C4	C9	-179.9(3)	C3	C1	C4	C9	0.0(5)	C1	C3	C7	C13	0.0(5)

C1	C4	C9	C13	0.1(5)	C3	C7	C13	C9	0.1(5)	C4	C9	C1	C7	-0.2(5)
C2	C1	C3	H8	0.0(14)	C4	C1	C3	H8	-179.9(13)	C2	C1	C4	H10	-0.1(14)
C3	C1	C4	H10	179.8(14)	O5	C2	N6	H11	-29.9(13)	O5	C2	N6	H12	-172.2(16)
C1	C2	N6	H11	153.8(12)	C1	C2	N6	H12	11.5(17)	C1	C3	C7	H14	179.7(12)
H8	C3	C7	C13	179.8(13)	H8	C3	C7	H14	-0.5(18)	C1	C4	C9	H15	-179.7(13)
H10	C4	C9	C13	-179.7(13)	H10	C4	C9	H15	0.5(19)	C3	C7	C13	H16	180.0(11)
H14	C7	C13	C9	-179.6(13)	H14	C7	C13	H16	0.3(17)	C4	C9	C13	H16	180.0(11)
H15	C9	C13	C7	179.6(13)	H15	C9	C13	H16	-0.2(18)					
C40	C38	C39	O42	169.0(6)	C40	C38	C39	N43	-4.0(7)	C41	C38	C39	O42	-11.1(7)
C41	C38	C39	N43	175.9(5)	C39	C38	C40	C44	179.7(3)	C41	C38	C40	C44	-0.2(5)
C39	C38	C41	C46	-179.8(3)	C40	C38	C41	C46	0.1(5)	C38	C40	C44	C50	0.2(5)
C38	C41	C46	C50	0.0(5)	C40	C44	C50	C46	0.0(5)	C41	C46	C50	C44	0.0(5)
C39	C38	C40	H45	-0.8(15)	C41	C38	C40	H45	179.3(14)	C39	C38	C41	H47	0.9(13)
C40	C38	C41	H47	-179.3(12)	O42	C39	N43	H48	-19.1(17)	O42	C39	N43	H49	-167(3)
C38	C39	N43	H48	153.8(14)	C38	C39	N43	H49	6(3)	C38	C40	C44	H51	179.7(12)
H45	C40	C44	C50	-179.4(13)	H45	C40	C44	H51	0.2(18)	C38	C41	C46	H52	180.0(13)
H47	C41	C46	C50	179.4(12)	H47	C41	C46	H52	-0.7(18)	C40	C44	C50	H53	-179.4(12)
H51	C44	C50	C46	-179.6(13)	H51	C44	C50	H53	1.0(18)	C41	C46	C50	H53	179.3(12)
H52	C46	C50	C44	180.0(13)	H52	C46	C50	H53	-0.7(18)					

S5. Geometric parameters of crystal structure from DFT calculation data.

O1	-	C1	1.2357	O2	-	C2	1.2518	N1	-	C1	1.4108	N1	-	C2	1.4084
N1	-	C7	1.4591	N2	-	C3	1.3813	N2	-	C4	1.3532	N3	-	C4	1.3455
N3	-	C5	1.3601	N4	-	C1	1.3873	N4	-	C5	1.3735	N4	-	C6	1.4622
C2	-	C3	1.4206	C3	-	C5	1.3937								
N2	-	H5	1.05	C4	-	H4	1.09	C6	-	H1	1.1	C6	-	H2	1.1
C6	-	H3	1.09	C7	-	H6	1.09	C7	-	H7	1.09	C7	-	H8	1.1
O3	-	C8	1.235	O4	-	C9	1.2578	N5	-	C8	1.413	N5	-	C9	1.4023
N5	-	C14	1.459	N6	-	C10	1.3814	N6	-	C11	1.3466	N7	-	C11	1.3476
N7	-	C12	1.3604	N8	-	C8	1.3882	N8	-	C12	1.3701	N8	-	C13	1.4619
C9	-	C10	1.4181	C10	-	C12	1.3929								
N6	-	H13	1.05	C11	-	H12	1.09	C13	-	H9	1.09	C13	-	H10	1.1
C13	-	H11	1.09	C14	-	H14	1.09	C14	-	H15	1.1	C14	-	H16	1.09
O5	-	C15	1.2632	N9	-	C15	1.3385	C15	-	C16	1.5001	C16	-	C17	1.4058
C16	-	C21	1.403	C17	-	C18	1.3967	C18	-	C19	1.3985	C19	-	C20	1.3971
C20	-	C21	1.3924												
N9	-	H17	1.03	N9	-	H18	1.03	C17	-	H23	1.09	C18	-	H22	1.09
C19	-	H21	1.09	C20	-	H20	1.09	C21	-	H19	1.09				
O6	-	C22	1.2606	N10	-	C22	1.3415	C22	-	C23	1.5027	C23	-	C24	1.4054
C23	-	C28	1.4031	C24	-	C25	1.3956	C25	-	C26	1.3976	C26	-	C27	1.3969
C27	-	C28	1.3941												
N10	-	H24	1.03	N10	-	H25	1.02	C24	-	H30	1.09	C25	-	H29	1.09
C26	-	H28	1.09	C27	-	H27	1.09	C28	-	H26	1.09				

C1	-	N1	-	C2	126.79	C1	-	N1	-	C7	116.14	C2	-	N1	-	C7	117.06
C3	-	N2	-	C4	106.29	C4	-	N3	-	C5	103.81	C1	-	N4	-	C5	119.77
C1	-	N4	-	C6	118.07	C5	-	N4	-	C6	122.13	O1	-	C1	-	N1	121.88
O1	-	C1	-	N4	121.34	N1	-	C1	-	N4	116.78	O2	-	C2	-	N1	120.68
O2	-	C2	-	C3	127.19	N1	-	C2	-	C3	112.13	N2	-	C3	-	C2	132.06
N2	-	C3	-	C5	105.31	C2	-	C3	-	C5	122.64	N2	-	C4	-	N3	113.26
N3	-	C5	-	N4	126.92	N3	-	C5	-	C3	111.32	N4	-	C5	-	C3	121.76
C3	-	N2	-	H5	126	C4	-	N2	-	H5	127	N2	-	C4	-	H4	124
N3	-	C4	-	H4	123	N4	-	C6	-	H1	110	N4	-	C6	-	H2	111
N4	-	C6	-	H3	108	H1	-	C6	-	H2	109	H1	-	C6	-	H3	110
H2	-	C6	-	H3	110	N1	-	C7	-	H6	109	N1	-	C7	-	H7	109
N1	-	C7	-	H8	111	H6	-	C7	-	H7	111	H6	-	C7	-	H8	109
H7	-	C7	-	H8	109												
C8	-	N5	-	C9	126.84	C8	-	N5	-	C14	116.84	C9	-	N5	-	C14	116.3
C1	-	N6	-	C11	106.59	C11	-	N7	-	C12	104.28	C8	-	N8	-	C12	119.79
C8	-	N8	-	C13	118.27	C12	-	N8	-	C13	121.91	O3	-	C8	-	N5	122.31
O3	-	C8	-	N8	121.25	N5	-	C8	-	N8	116.44	O4	-	C9	-	N5	120.61
O4	-	C9	-	C10	126.74	N5	-	C9	-	C10	112.65	N6	-	C10	-	C9	132.47
N6	-	C10	-	C12	105.46	C9	-	C10	-	C12	122.07	N6	-	C11	-	N7	112.87
N7	-	C12	-	N8	127.07	N7	-	C12	-	C10	110.8	N8	-	C12	-	C10	122.14
C10	-	N6	-	H13	127	C11	-	N6	-	H13	126	N6	-	C11	-	H12	124
N7	-	C11	-	H12	123	N8	-	C13	-	H9	109	N8	-	C13	-	H10	111
N8	-	C13	-	H11	109	H9	-	C13	-	H10	109	H9	-	C13	-	H11	110
H10	-	C13	-	H11	109	N5	-	C14	-	H14	109	N5	-	C14	-	H15	110
N5	-	C14	-	H16	110	H14	-	C14	-	H15	110	H14	-	C14	-	H16	109
H15	-	C14	-	H16	108												
O5	-	C15	-	N9	121.8	O5	-	C15	-	C16	119.53	N9	-	C15	-	C16	118.66
C15	-	C16	-	C17	123.14	C15	-	C16	-	C21	118.01	C17	-	C16	-	C21	118.81
C16	-	C17	-	C18	120.32	C17	-	C18	-	C19	120.47	C18	-	C19	-	C20	119.29
C19	-	C20	-	C21	120.45	C16	-	C21	-	C20	120.64						
C15	-	N9	-	H17	119	C15	-	N9	-	H18	124	H17	-	N9	-	H18	117
C16	-	C17	-	H23	120	C18	-	C17	-	H23	119	C17	-	C18	-	H22	120
C19	-	C18	-	H22	120	C18	-	C19	-	H21	121	C20	-	C19	-	H21	120
C19	-	C20	-	H20	120	C21	-	C20	-	H20	120	C16	-	C21	-	H19	119
C20	-	C21	-	H19	121												
O6	-	C22	-	N10	121.78	O6	-	C22	-	C23	119.69	N10	-	C22	-	C23	118.51
C22	-	C23	-	C24	123.35	C22	-	C23	-	C28	117.95	C24	-	C23	-	C28	118.64
C23	-	C24	-	C25	120.37	C24	-	C25	-	C26	120.46	C25	-	C26	-	C27	119.55
C26	-	C27	-	C28	120.02	C23	-	C28	-	C27	120.95						
C22	-	N10	-	H24	119	C22	-	N10	-	H25	124	H24	-	N10	-	H25	117
C23	-	C24	-	H30	121	C25	-	C24	-	H30	119	C24	-	C25	-	H29	121
C26	-	C25	-	H29	119	C25	-	C26	-	H28	120	C27	-	C26	-	H28	120
C26	-	C27	-	H27	120	C28	-	C27	-	H27	120	C23	-	C28	-	H26	118
C27	-	C28	-	H26	121												

C2	N1	C1	O1	-175.82	C2	N1	C1	N4	4.36	C7	N1	C1	O1	2.92
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C7	N1	C1	N4	-176.9	C1	N1	C2	O2	176.29	C1	N1	C2	C3	-4.1
C7	N1	C2	O2	-2.44	C7	N1	C2	C3	177.17	C4	N2	C3	C2	179.98
C4	N2	C3	C5	0	C3	N2	C4	N3	0.37	C5	N3	C4	N2	-0.6
C4	N3	C5	N4	-179.57	C4	N3	C5	C3	0.59	C5	N4	C1	O1	178.03
C5	N4	C1	N1	-2.14	C6	N4	C1	O1	-0.15	C6	N4	C1	N1	179.68
C1	N4	C5	N3	-179.53	C1	N4	C5	C3	0.3	C6	N4	C5	N3	-1.42
C6	N4	C5	C3	178.4	O2	C2	C3	N2	1.51	O2	C2	C3	C5	-178.53
N1	C2	C3	N2	-178.07	N1	C2	C3	C5	1.9	N2	C3	C5	N3	-0.39
N2	C3	C5	N4	179.77	C2	C3	C5	N3	179.64	C2	C3	C5	N4	-0.2
C1	N1	C7	H6	30	C1	N1	C7	H7	152	C1	N1	C7	H8	-89
C2	N1	C7	H6	-151	C2	N1	C7	H7	-29	C2	N1	C7	H8	90
H5	N2	C3	C2	5	H5	N2	C3	C5	-174	C3	N2	C4	H4	-179
H5	N2	C4	N3	175	H5	N2	C4	H4	-4	C5	N3	C4	H4	179
C1	N4	C6	H1	52	C1	N4	C6	H2	-67	C1	N4	C6	H3	172
C5	N4	C6	H1	-126	C5	N4	C6	H2	114	C5	N4	C6	H3	-6
C9	N5	C8	O3	177.59	C9	N5	C8	N8	-2.83	C14	N5	C8	O3	-1.15
C14	N5	C8	N8	178.42	C8	N5	C9	O4	-179.27	C8	N5	C9	C10	0.83
C14	N5	C9	O4	-0.52	C14	N5	C9	C10	179.57	C11	N6	C10	C9	-179.17
C11	N6	C10	C12	0.09	C10	N6	C11	N7	-0.47	C12	N7	C11	N6	0.65
C11	N7	C12	N8	178.95	C11	N7	C12	C10	-0.58	C12	N8	C8	O3	-177.03
C12	N8	C8	N5	3.39	C13	N8	C8	O3	0.99	C13	N8	C8	N5	-178.59
C8	N8	C12	N7	178.28	C8	N8	C12	C10	-2.24	C13	N8	C12	N7	0.33
C13	N8	C12	C10	179.81	O4	C9	C10	N6	-0.15	O4	C9	C10	C12	-179.31
N5	C9	C10	N6	179.75	N5	C9	C10	C12	0.59	N6	C10	C12	N7	0.32
N6	C10	C12	N8	-179.24	C9	C1	C12	N7	179.67	C9	C10	C12	N8	0.12
C8	N5	C14	H14	-6	C8	N5	C14	H15	114	C8	N5	C14	H16	-126
C9	N5	C14	H14	175	C9	N5	C14	H15	-65	C9	N5	C14	H16	55
H13	N6	C10	C9	-3	H13	N6	C10	C12	176	C10	N6	C11	H12	-180
H13	N6	C11	N7	-177	H13	N6	C11	H12	4	C12	N7	C11	H12	-180
C8	N8	C13	H9	41	C8	N8	C13	H10	-80	C8	N8	C13	H11	160
C12	N8	C13	H9	-141	C12	N8	C13	H10	98	C12	N8	C13	H11	-22
O5	C15	C16	C17	-165.87	O5	C15	C16	C21	11.8	N9	C15	C16	C17	12.56
N9	C15	C16	C21	-169.77	C15	C16	C17	C18	177.65	C21	C16	C17	C18	0
C15	C16	C21	C20	-178.27	C17	C16	C21	C20	-0.5	C16	C17	C18	C19	0.35
C17	C18	C19	C20	-0.2	C18	C19	C20	C21	-0.29	C19	C20	C21	C16	0.65
H17	N9	C15	O5	4	H17	N9	C15	C16	-175	H18	N9	C15	O5	-172
H18	N9	C15	C16	10	C15	C16	C17	H23	-2	C21	C16	C17	H23	-180
C15	C16	C21	H19	1	C17	C16	C21	H19	179	C16	C17	C18	H22	-179
H23	C17	C18	C19	-180	H23	C17	C18	H22	0	C17	C18	C19	H21	180
H22	C18	C19	C20	180	H22	C18	C19	H21	0	C18	C19	C20	H20	180
H21	C19	C20	C21	180	H21	C19	C20	H20	0	C19	C20	C21	H19	-179
H20	C20	C21	C16	-179	H20	C20	C21	H19	1					
O6	C22	C23	C24	172.95	O6	C22	C23	C28	-4.39	N10	C22	C23	C24	-5.57
N10	C22	C23	C28	177.09	C22	C23	C24	C25	-177.39	C28	C23	C24	C25	-0.06
C22	C23	C28	C27	177.7	C24	C23	C28	C27	0.23	C23	C24	C25	C26	-0.03
C24	C25	C26	C27	-0.02	C25	C26	C27	C28	0.18	C26	C27	C28	C23	-0.29

H24 N10 C22 O6 -3	H24 N10 C22 C23 175	H25 N10 C22 O6) 179
H25 N10 C22 C23 -3	C22 C23 C24 H30 1	C28 C23 C24 H30 179
C22 C23 C28 H26 -1	C24 C23 C28 H26 -179	C23 C24 C25 H29 178
H30 C24 C25 C26 -179	H30 C24 C25 H29 -1	C24 C25 C26 H28 179
H29 C25 C26 C27 -178	H29 C25 C26 H28 1	C25 C26 C27 H27 180
H28 C26 C27 C28 -179	H28 C26 C27 H27 1	C26 C27 C28 H26 179
H27 C27 C28 C23 -180	H27 C27 C28 H26 -1	
