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Supporting information for article:

Solvomorphs of tyraminium 5,5-diethylbarbiturate: a rare example of the barbiturate *R*3^3(12) hydrogen-bond motif and a crystal structure with *Z*′ = 4

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S1. Tyraminium 5,5-diethylbarbiturate (I)

Computing details:

Data collection: *CrysAlisPro 1.171.38.34a* (Rigaku OD, 2015); cell refinement: *CrysAlisPro 1.171.38.34a* (Rigaku OD, 2015), data reduction: *CrysAlisPro 1.171.38.34a* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXT 2014/5* (Sheldrick, 2014); program(s) used to refine structure: *SHELXL-2018/3* (Sheldrick, 2015) in WinGX (Farrugia, 2012); molecular graphics: *ORTEP-3* (Farrugia, 1997) and Mercury 3.10.2 (Macrae *et al*., 2008); software used to prepare material for publication: SHELXL-2018/3 (Sheldrick, 2015).

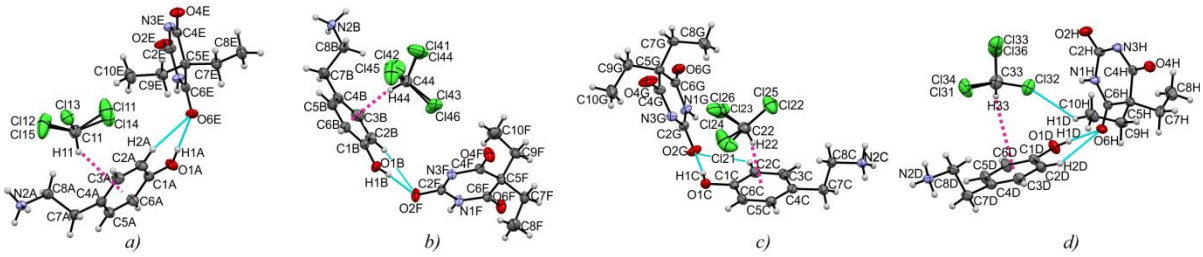

Figure S1 Four independent moieties of tyraminium barbitalate ions and chloroform molecules in the asymmetric unit of (I) (a-d).

Table S1 Hydrogen-bond geometry (Å,°) for (I).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*B*—H1*B*···O2*F*	0.80 (2)	1.80 (2)	2.597 (1)	173 (2)
O1*C*—H1*C*···O2*G*	0.80 (2)	1.82 (2)	2.617 (1)	176 (2)
O1*D*—H1*D*···O6*H*	0.81 (2)	1.88 (2)	2.694 (1)	177 (2)
O1*A*—H1*A*···O6*E*	0.79 (2)	1.92 (2)	2.705 (1)	175 (2)
N2*C*—H13*C*···N3*E*^{ii}	0.91 (1)	1.97 (1)	2.863 (2)	165 (2)
N2*B*—H12*B*···N3*H*^{iv}	0.92 (1)	2.00 (1)	2.893 (2)	166 (2)
N2*D*—H12*D*···N3*G*^{iv}	0.90 (1)	2.03 (1)	2.856 (2)	153 (1)
N2*A*—H12*A*···N3*F*^{ii}	0.91 (1)	2.06 (1)	2.893 (2)	153 (2)
N2*D*—H11*D*···O4*G*	0.90 (1)	1.82 (1)	2.722 (2)	174 (2)

N2*A*—H13*A*···O4*F*	0.91 (1)	1.83 (1)	2.727 (2)	170
N1*F*—H1*F*···O2*G*	0.88 (1)	1.88 (1)	2.759 (1)	175 (2)
N1*G*—H1*G*···O2*F*	0.88 (1)	1.89 (1)	2.770 (1)	175 (2)
N1*E*—H1*E*···O2*H*^{xi}	0.88 (1)	1.93 (1)	2.805 (2)	173 (2)
N1*H*—H1*H*···O2*E*^{xii}	0.88 (1)	1.95 (1)	2.812 (2)	170 (2)
N2*B*—H11*B*···O1*A*^{v}	0.91 (1)	1.97 (1)	2.842 (2)	161 (2)
N2*D*—H13*D*···O4*E*^{x}	0.90 (1)	1.98 (1)	2.798 (2)	149 (1)
N2*C*—H11*C*···O1*D*^{viii}	0.91 (1)	1.99 (1)	2.860 (2)	160 (2)
N2*A*—H11*A*···O4*H*^{i}	0.91 (1)	2.00 (1)	2.837 (1)	153 (2)
N2*C*—H12*C*···O6*F*^{ix}	0.91 (1)	2.06 (1)	2.778 (2)	135 (1)
N2*B*—H13*B*···O6*G*^{vi}	0.91 (1)	2.11 (1)	2.794 (2)	131 (1)
N2*B*—H13*B*···O1*B*^{vi}	0.91 (1)	2.36 (1)	2.970 (2)	124 (1)
N2*C*—H12*C*···O1*C*^{ix}	0.91 (1)	2.42 (2)	2.962 (2)	118 (1)
C8*B*—H8*B*1···O2*H*^{iv}	0.99	2.52	3.096 (2)	117
C7*A*—H7*A*1···O4*F*	0.99	2.60	3.321 (2)	130
C2*A*—H2*A*···O6*E*	0.95	2.69	3.346	127
C2*D*—H2*D*···O6*H*	0.95	2.72	3.366	126
C2*C*—H2*C*···O2*G*	0.95	2.74	3.378	125
C2*B*—H2*B*···O2*F*	0.95	2.89	3.489	122
C6*C*—H6*C*···N3*E*^{vii}	0.95	2.66	3.477 (2)	145
C6*B*—H6*B*···N3*H*^{iii}	0.95	2.69	3.519 (2)	146
N2A—H12A···Cl46^{xiii}	0.88	3.04	3.593	123
N2A—H12A···Cl43^{xiii}	0.88	3.10	3.719	130
N2D—H12D···Cl24^{xiv}	0.87	3.11	3.682	125
N2D—H12D···Cl21^{xiv}	0.87	3.19	3.820	131
N1H—H1H···Cl32^{iv}	0.86	3.32	3.438	91

N1G—H1G···Cl15^{viii}	0.91	3.33	3.479	92
N1G—H1G···Cl12^{viii}	0.91	3.44	3.564	90
C10*H*—H10*H*···Cl32^{iv}	0.99	2.84	3.649	140
C5*B*—H5*B*···Cl15^{iii}	0.95	2.86	3.740	155
C5*B*—H5*B*···Cl12^{iii}	0.95	2.87	3.765	157
C8*F*—H83*F*···Cl13^{viii}	0.98	2.95	3.463	114
C10*H*—H12*H*···Cl23^{viii}	0.98	2.96	3.930	170
C8*F*—H82*F*···Cl45^{xiii}	0.98	3.03	3.698	126
C10*H*—H12*H*···Cl26^{viii}	0.98	3.03	3.984	164
C10*G*—H10*G*···Cl42^{vii}	0.98	3.03	3.892	148
C7*C*—H71*C*···Cl34^{ix}	0.99	3.04	3.972	158
C10*E*—H10*E*···Cl13^{xi}	0.98	3.04	3.618	119
C10*G*—H10*G*···Cl45^{vii}	0.98	3.04	3.914	149
C10*G*—H11*G*···Cl15^{viii}	0.98	3.05	3.815	136
C10*G*—H11*G*···Cl12^{viii}	0.98	3.06	3.792	133
C10*F*—H11*F*···Cl43^{v}	0.98	3.06	4.022	168
C3*B*—H3*B*···Cl32	0.99	3.07	4.958	156
C5*C*—H5*C*···Cl33^{ix}	0.95	3.07	3.074	134
C3*D*—H3*D*···Cl24^{viii}	0.95	3.09	4.018	167
C7*C*—H71*C*···Cl31^{ix}	0.99	3.09	4.028	159
C8*F*—H81*F*···Cl13^{viii}	0.98	3.10	3.463	103
C8*E*—H82*E*···Cl33^{v}	0.99	3.11	3.917	130
C7*G*—H72*G*···Cl26^{xiv}	0.99	3.12	3.893	136
C8*E*—H82*E*···Cl36^{v}	0.99	3.13	3.902	136
C8*F*—H82*F*···Cl42^{xiii}	0.98	3.17	3.836	126
C10*F*—H11*F*···Cl46^{v}	0.98	3.30	4.264	172

C10*E*—H12*E*···Cl13^{xi}	0.98	3.37	3.618	97

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) *x*+1/2, −*y*+3/2, *z*−1/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+1, −*y*, −*z*; (vi) −*x*+3/2, *y*−1/2, −*z*+1/2; (vii) *x*−1/2, −*y*+1/2, *z*+1/2; (viii) −*x*+1, −*y*+2, −*z*+1; (ix) −*x*+1/2, *y*+1/2, −*z*+1/2; (x) −*x*+3/2, *y*+1/2, −*z*+1/2; (xi) *x*, *y*−1, *z*−1; (xii) *x*, *y*+1, *z*+1; (xiii) *x*, *y*+1, *z*; (xiv) *x*, *y*-1, *z*

Table S2 The geometry of C-H···π interactions (Å,°) for (I).

C – H···π	D – H	H – A	D – A	∢D – H···A
C11-H11···Cg(C1A^C6A)	0.93	3.23	3.890	130
C22-H22··· Cg(C1C^C6C)	0.93	2.54	3.447	165
C33-H33··· Cg(C1D^C6D)	0.97	3.57	4.177	123
C44-H44··· Cg(C1B^C6B)	0.98	2.49	3.449	168
C6A-H6A··· Cg(C1B^C6B)	0.95	3.05	3.730	130
C2D-H2D··· Cg(C1C^C6C)	0.95	3.08	3.774	131

Table S3 Fractional atomic coordinates and equivalent isotropic displacement parameters of (I) as well as site occupancy factors where needed (Occ.) (Å^2).

	x	y	z	U_{iso}^*/U_{eq}	Occ. (<1)
C1A	0.36861(7)	0.12333(8)	-0.11878(6)	0.0244(3)	
O1A	0.37299(5)	0.05132(6)	-0.13698(4)	0.0310(2)	
H1A	0.4107(10)	0.0344(11)	-0.1272(7)	0.037*	
C2A	0.42134(7)	0.15582(8)	-0.07881(6)	0.0284(3)	
H2A	0.462194	0.127879	-0.062912	0.034*	
C3A	0.41379(8)	0.22945(9)	-0.06234(6)	0.0313(3)	
H3A	0.449918	0.251429	-0.035047	0.038*	

C4A	0.35442(7)	0.27184(8)	-0.08495(6)	0.0261(3)
C5A	0.30217(7)	0.23780(8)	-0.12436(6)	0.0285(3)
H5A	0.261043	0.265472	-0.139967	0.034*
C6A	0.30861(7)	0.16445(8)	-0.14144(6)	0.0295(3)
H6A	0.272261	0.142350	-0.168482	0.035*
C7A	0.34846(8)	0.35298(8)	-0.06836(6)	0.0301(3)
H7A1	0.365614	0.357609	-0.028610	0.036*
H7A2	0.298976	0.368649	-0.078460	0.036*
C8A	0.39076(7)	0.40441(8)	-0.09596(6)	0.0263(3)
H8A1	0.439983	0.387799	-0.086287	0.032*
H8A2	0.373147	0.399756	-0.135669	0.032*
N2A	0.38714(6)	0.48488(6)	-0.08021(5)	0.0210(2)
H11A	0.3435(6)	0.5030(9)	-0.0932(7)	0.031*
H12A	0.4204(7)	0.5103(9)	-0.0918(7)	0.031*
H13A	0.3969(9)	0.4853(10)	-0.0435(4)	0.031*
C1B	0.67898(7)	0.37382(8)	0.20361(5)	0.0227(3)
O1B	0.66249(5)	0.44645(6)	0.18814(4)	0.0251(2)
H1B	0.6255(9)	0.4584(10)	0.1934(7)	0.030*
C2B	0.63999(8)	0.32984(9)	0.23086(6)	0.0302(3)
H2B	0.599185	0.349828	0.238860	0.036*
C3B	0.66135(8)	0.25661(9)	0.24617(6)	0.0336(3)
H3B	0.634581	0.226988	0.264657	0.040*
C4B	0.72094(8)	0.22547(8)	0.23515(6)	0.0300(3)
C5B	0.75851(7)	0.26987(8)	0.20737(6)	0.0304(3)
H5B	0.798916	0.249630	0.198868	0.036*
C6B	0.73808(7)	0.34334(8)	0.19178(6)	0.0275(3)
H6B	0.764638	0.372741	0.172987	0.033*
C7B	0.74273(9)	0.14538(9)	0.25192(7)	0.0357(3)
H7B1	0.734661	0.135169	0.288043	0.043*

H7B2	0.793103	0.139258	0.254489	0.043*
C8B	0.70187(7)	0.08948(8)	0.21139(6)	0.0245(3)
H8B1	0.651463	0.100252	0.204944	0.029*
H8B2	0.715021	0.094858	0.176568	0.029*
N2B	0.71618(6)	0.01076(6)	0.23188(5)	0.0215(2)
H11B	0.6860(7)	-0.0171(9)	0.2067(6)	0.032*
H12B	0.7074(9)	0.0060(10)	0.2653(4)	0.032*
H13B	0.7608(5)	-0.0032(9)	0.2336(7)	0.032*
C1C	0.31853(7)	0.63016(7)	0.29378(5)	0.0217(3)
O1C	0.33471(5)	0.55846(5)	0.31199(4)	0.0248(2)
H1C	0.3715(9)	0.5464(10)	0.3067(7)	0.030*
C2C	0.35778(7)	0.67050(8)	0.26487(6)	0.0266(3)
H2C	0.397580	0.648023	0.256829	0.032*
C3C	0.33859(7)	0.74364(8)	0.24784(6)	0.0289(3)
H3C	0.365784	0.770710	0.228261	0.035*
C4C	0.28039(7)	0.77824(8)	0.25880(6)	0.0262(3)
C5C	0.24167(7)	0.73693(8)	0.28758(6)	0.0268(3)
H5C	0.201872	0.759443	0.295609	0.032*
C6C	0.25981(7)	0.66365(8)	0.30483(6)	0.0248(3)
H6C	0.232335	0.636425	0.324095	0.030*
C7C	0.26178(8)	0.85881(8)	0.24229(6)	0.0302(3)
H7C1	0.211513	0.867037	0.239130	0.036*
H7C2	0.270984	0.868513	0.206472	0.036*
C8C	0.30401(7)	0.91336(8)	0.28358(6)	0.0246(3)
H8C1	0.294514	0.903901	0.319334	0.030*
H8C2	0.354279	0.904823	0.286959	0.030*
N2C	0.28615(6)	0.99288(6)	0.26716(5)	0.0213(2)
H11C	0.3159(7)	1.0201(9)	0.2930(6)	0.032*
H12C	0.2412(5)	1.0021(10)	0.2679(7)	0.032*

H13C	0.2935(9)	1.0006(10)	0.2337(4)	0.032*
C1D	0.62991(7)	0.87937(8)	0.61406(6)	0.0255(3)
O1D	0.62634(5)	0.95053(6)	0.63429(4)	0.0320(2)
H1D	0.5876(10)	0.9685(11)	0.6244(8)	0.038*
C2D	0.57738(7)	0.84983(8)	0.57256(6)	0.0282(3)
H2D	0.537519	0.879321	0.556707	0.034*
C3D	0.58372(8)	0.77675(9)	0.55448(6)	0.0309(3)
H3D	0.547583	0.756598	0.526307	0.037*
C4D	0.64191(7)	0.73226(8)	0.57674(6)	0.0275(3)
C5D	0.69429(8)	0.76385(9)	0.61736(6)	0.0320(3)
H5D	0.734728	0.734947	0.632698	0.038*
C6D	0.68886(8)	0.83653(9)	0.63599(6)	0.0323(3)
H6D	0.725381	0.857027	0.663708	0.039*
C7D	0.64576(8)	0.65100(8)	0.55966(6)	0.0306(3)
H7D1	0.695083	0.635388	0.565921	0.037*
H7D2	0.623520	0.645782	0.520566	0.037*
C8D	0.60876(8)	0.60069(8)	0.59204(6)	0.0287(3)
H8D1	0.629757	0.608529	0.631094	0.034*
H8D2	0.559216	0.615863	0.584597	0.034*
N2D	0.61273(6)	0.51898(7)	0.57921(5)	0.0216(2)
H11D	0.6020(9)	0.5139(10)	0.5429(4)	0.032*
H12D	0.5802(7)	0.4951(9)	0.5921(7)	0.032*
H13D	0.6564(6)	0.5008(9)	0.5917(7)	0.032*
N1E	0.54458(6)	-0.01240(7)	-0.17213(5)	0.0228(2)
H1E	0.5035(6)	-0.0149(9)	-0.1948(6)	0.027*
C2E	0.59888(7)	-0.01323(8)	-0.19839(6)	0.0254(3)
O2E	0.58221(5)	-0.01958(8)	-0.24838(4)	0.0408(3)
N3E	0.66579(6)	-0.00755(7)	-0.17063(5)	0.0236(2)
C4E	0.68281(7)	-0.00195(7)	-0.11621(5)	0.0216(3)

O4E	0.74413(5)	0.00157(7)	-0.09019(4)	0.0325(2)
C5E	0.62721(6)	0.00203(7)	-0.08349(5)	0.0209(2)
C6E	0.55330(6)	-0.00505(7)	-0.11807(5)	0.0201(2)
O6E	0.50308(5)	-0.00342(6)	-0.09768(4)	0.0260(2)
C7E	0.64044(7)	-0.06074(8)	-0.04021(6)	0.0282(3)
H7E1	0.686220	-0.051711	-0.014711	0.034*
H7E2	0.604453	-0.057217	-0.019437	0.034*
C8E	0.63970(10)	-0.14044(9)	-0.06283(8)	0.0397(4)
H81E	0.6759(9)	-0.1457(12)	-0.0827(8)	0.060*
H82E	0.5938(7)	-0.1528(12)	-0.0865(7)	0.060*
H83E	0.6478(11)	-0.1775(10)	-0.0333(6)	0.060*
C9E	0.63357(8)	0.07983(8)	-0.05473(6)	0.0287(3)
H9E1	0.599662	0.081842	-0.032030	0.034*
H9E2	0.680777	0.084271	-0.030385	0.034*
C10E	0.62097(10)	0.14696(9)	-0.09309(8)	0.0408(4)
H10E	0.5744(6)	0.1466(12)	-0.1173(7)	0.061*
H11E	0.6532(9)	0.1482(12)	-0.1165(7)	0.061*
H12E	0.6242(11)	0.1936(8)	-0.0724(8)	0.061*
N1F	0.42888(6)	0.50181(7)	0.18497(4)	0.0244(2)
H1F	0.4345(9)	0.5060(9)	0.2203(4)	0.029*
C2F	0.48900(7)	0.49390(8)	0.16679(5)	0.0220(3)
O2F	0.54524(5)	0.49721(7)	0.20212(4)	0.0330(2)
N3F	0.48712(6)	0.48364(7)	0.11463(4)	0.0221(2)
C4F	0.42511(7)	0.48047(8)	0.07772(5)	0.0228(3)
O4F	0.42386(6)	0.47125(7)	0.02967(4)	0.0382(3)
C5F	0.35504(7)	0.48650(8)	0.09310(5)	0.0223(3)
C6F	0.36314(7)	0.49848(8)	0.15328(5)	0.0227(3)
O6F	0.31285(5)	0.50441(7)	0.17279(4)	0.0333(2)
C7F	0.31193(7)	0.55249(9)	0.06233(6)	0.0293(3)

H7F1	0.304689	0.543735	0.022995	0.035*
H7F2	0.265586	0.552569	0.070448	0.035*
C8F	0.34512(10)	0.62998(10)	0.07608(8)	0.0433(4)
H81F	0.3901(7)	0.6317(13)	0.0665(9)	0.065*
H83F	0.3505(11)	0.6431(13)	0.1142(5)	0.065*
H82F	0.3155(10)	0.6691(10)	0.0547(8)	0.065*
C9F	0.31394(7)	0.41235(9)	0.07711(6)	0.0307(3)
H9F1	0.268229	0.416970	0.085998	0.037*
H9F2	0.305119	0.405549	0.037469	0.037*
C10F	0.35083(10)	0.34251(10)	0.10497(9)	0.0459(4)
H10F	0.3608(12)	0.3474(13)	0.1445(4)	0.069*
H11F	0.3940(8)	0.3329(13)	0.0941(9)	0.069*
H12F	0.3231(10)	0.2963(8)	0.0957(9)	0.069*
N1G	0.56928(6)	0.49797(7)	0.31382(4)	0.0229(2)
H1G	0.5641(9)	0.4992(9)	0.2784(4)	0.027*
C2G	0.50907(6)	0.50621(7)	0.33189(5)	0.0204(2)
O2G	0.45327(5)	0.51142(6)	0.29605(4)	0.0301(2)
N3G	0.51008(6)	0.50865(7)	0.38419(4)	0.0217(2)
C4G	0.57128(7)	0.49991(8)	0.42173(5)	0.0251(3)
O4G	0.57145(6)	0.50160(9)	0.46992(4)	0.0497(4)
C5G	0.64069(7)	0.48661(8)	0.40685(5)	0.0221(3)
C6G	0.63423(7)	0.48944(8)	0.34636(5)	0.0213(2)
O6G	0.68484(5)	0.48377(6)	0.32717(4)	0.0305(2)
C7G	0.66950(8)	0.40825(9)	0.42806(6)	0.0321(3)
H7G1	0.716157	0.401814	0.421122	0.039*
H7G2	0.675233	0.406741	0.467719	0.039*
C8G	0.62353(12)	0.34225(10)	0.40254(8)	0.0481(5)
H83G	0.5778(7)	0.3463(13)	0.4103(9)	0.072*
H82G	0.6158(12)	0.3385(13)	0.3633(4)	0.072*

H81G	0.6446(11)	0.2944(8)	0.4167(9)	0.072*
C9G	0.69306(7)	0.54798(8)	0.43409(6)	0.0272(3)
H9G1	0.699405	0.544818	0.473759	0.033*
H9G2	0.738658	0.537417	0.426275	0.033*
C10G	0.67099(9)	0.62782(10)	0.41575(7)	0.0386(4)
H10G	0.7044(9)	0.6638(10)	0.4370(7)	0.058*
H11G	0.6705(11)	0.6345(12)	0.3775(4)	0.058*
H12G	0.6245(7)	0.6386(12)	0.4213(8)	0.058*
N1H	0.45599(6)	0.99824(7)	0.67287(5)	0.0226(2)
H1H	0.4976(5)	0.9923(9)	0.6943(6)	0.027*
C2H	0.40152(7)	0.99296(8)	0.69890(5)	0.0225(3)
O2H	0.41817(5)	0.98367(7)	0.74855(4)	0.0325(2)
N3H	0.33437(5)	0.99736(6)	0.67115(4)	0.0217(2)
C4H	0.31752(6)	1.00982(7)	0.61710(5)	0.0206(2)
O4H	0.25619(5)	1.01552(6)	0.59123(4)	0.0281(2)
C5H	0.37361(6)	1.01868(8)	0.58497(5)	0.0217(3)
C6H	0.44720(6)	1.00766(7)	0.61896(5)	0.0197(2)
O6H	0.49736(5)	1.00817(6)	0.59835(4)	0.0255(2)
C7H	0.36888(8)	1.09914(9)	0.56058(7)	0.0329(3)
H7H1	0.402574	1.103161	0.537804	0.040*
H7H2	0.321675	1.106323	0.536738	0.040*
C8H	0.38322(10)	1.16237(10)	0.60215(9)	0.0453(4)
H83H	0.3507(10)	1.1608(13)	0.6256(8)	0.068*
H81H	0.4301(7)	1.1601(13)	0.6267(8)	0.068*
H82H	0.3812(11)	1.2130(7)	0.5863(8)	0.068*
C9H	0.35930(7)	0.96051(9)	0.53852(6)	0.0301(3)
H9H1	0.312488	0.970257	0.514744	0.036*
H9H2	0.393682	0.968062	0.516671	0.036*
C10H	0.36276(9)	0.87869(10)	0.55718(8)	0.0392(4)

H10H	0.4102(6)	0.8639(12)	0.5769(8)	0.059*	
H11H	0.3303(9)	0.8692(12)	0.5801(7)	0.059*	
H12H	0.3498(10)	0.8444(10)	0.5261(6)	0.059*	
C11	0.44411(9)	1.25688(10)	0.78116(8)	0.0418(4)	
H11	0.4020(10)	1.2598(11)	0.7906(8)	0.050*	
Cl11	0.4528(2)	1.1606(2)	0.77201(16)	0.0450(8)	0.64(3)
Cl12	0.43915(14)	1.3065(2)	0.72001(14)	0.0528(10)	0.64(3)
Cl13	0.51153(2)	1.29464(3)	0.83282(2)	0.04587(11)	
Cl14	0.4675(13)	1.1630(5)	0.7679(5)	0.077(2)	0.36(3)
Cl15	0.4362(4)	1.3129(6)	0.7238(4)	0.093(3)	0.36(3)
C22	0.60541(9)	1.25626(10)	0.59427(7)	0.0373(4)	
H22	0.6300(10)	1.2573(11)	0.6302(8)	0.045*	
Cl21	0.53840(19)	1.3222(2)	0.58980(13)	0.0588(5)	0.66(2)
Cl22	0.56954(18)	1.16469(18)	0.58074(18)	0.0444(6)	0.66(2)
Cl23	0.66780(18)	1.2756(2)	0.55699(12)	0.0586(6)	0.66(2)
Cl24	0.5414(4)	1.3264(4)	0.5735(9)	0.084(3)	0.34(2)
Cl25	0.5753(4)	1.1663(4)	0.5758(4)	0.0619(18)	0.34(2)
Cl26	0.6554(8)	1.2861(6)	0.5518(4)	0.0811(18)	0.34(2)
C33	0.44699(9)	0.23011(10)	0.27147(7)	0.0400(4)	
H33	0.4042(10)	0.2090(11)	0.2764(8)	0.048*	
Cl31	0.4443(3)	0.3301(3)	0.2752(3)	0.0440(10)	0.49(3)
Cl32	0.51752(2)	0.19366(3)	0.32079(2)	0.04835(11)	
Cl33	0.4454(5)	0.2018(4)	0.2075(2)	0.0482(8)	0.49(3)
Cl34	0.4417(3)	0.3275(3)	0.2792(3)	0.0519(10)	0.51(3)
Cl36	0.4627(8)	0.2091(3)	0.2057(2)	0.0525(12)	0.51(3)
C44	0.39485(9)	-0.24985(10)	-0.09139(7)	0.0398(4)	
H44	0.3687(10)	-0.2556(11)	-0.1289(8)	0.048*	
Cl41	0.43767(11)	-0.15986(15)	-0.08628(13)	0.0519(6)	0.65(2)
Cl42	0.3386(2)	-0.2515(3)	-0.05091(13)	0.0824(8)	0.65(2)

Cl43	0.45674(14)	-0.32033(17)	-0.0816(3)	0.0590(7)	0.65(2)
Cl44	0.4298(5)	-0.1651(4)	-0.0766(4)	0.0866(18)	0.35(2)
Cl45	0.3289(4)	-0.2675(7)	-0.0527(2)	0.0771(17)	0.35(2)
Cl46	0.4545(3)	-0.3260(4)	-0.0626(4)	0.0584(12)	0.35(2)

Table S4 Atomic displacement parameters of (I) (Å^2).

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1A	0.0226(6)	0.0234(7)	0.0278(7)	-0.0033(5)	0.0073(5)	-0.0004(5)
O1A	0.0237(5)	0.0254(5)	0.0403(6)	-0.0089(4)	0.0011(4)	0.0031(4)
C2A	0.0228(6)	0.0308(8)	0.0298(7)	-0.0045(6)	0.0029(5)	0.0012(5)
C3A	0.0282(7)	0.0313(8)	0.0328(8)	-0.0086(6)	0.0047(6)	-0.0034(6)
C4A	0.0295(7)	0.0241(7)	0.0284(7)	-0.0027(5)	0.0139(6)	-0.0027(5)
C5A	0.0260(7)	0.0250(7)	0.0341(8)	0.0010(6)	0.0065(6)	0.0035(5)
C6A	0.0248(7)	0.0280(7)	0.0319(7)	-0.0047(6)	-0.0001(6)	0.0003(5)
C7A	0.0332(7)	0.0245(7)	0.0375(8)	-0.0054(6)	0.0182(6)	-0.0027(6)
C8A	0.0306(7)	0.0244(7)	0.0268(7)	-0.0043(5)	0.0126(6)	-0.0004(5)
N2A	0.0205(5)	0.0244(6)	0.0182(5)	-0.0013(4)	0.0052(4)	-0.0006(4)
C1B	0.0209(6)	0.0243(7)	0.0217(6)	-0.0002(5)	0.0029(5)	-0.0027(5)
O1B	0.0194(4)	0.0264(5)	0.0302(5)	0.0032(4)	0.0075(4)	0.0031(4)
C2B	0.0290(7)	0.0327(8)	0.0318(8)	-0.0005(6)	0.0130(6)	-0.0036(6)
C3B	0.0390(8)	0.0312(8)	0.0324(8)	0.0037(6)	0.0121(6)	-0.0089(6)
C4B	0.0337(7)	0.0232(7)	0.0290(7)	0.0005(6)	-0.0001(6)	-0.0056(6)
C5B	0.0246(7)	0.0265(7)	0.0389(8)	0.0013(6)	0.0056(6)	-0.0007(5)
C6B	0.0235(6)	0.0250(7)	0.0350(8)	0.0023(6)	0.0091(6)	-0.0032(5)
C7B	0.0408(9)	0.0246(7)	0.0349(8)	0.0041(6)	-0.0037(7)	-0.0055(6)
C8B	0.0245(6)	0.0239(7)	0.0246(7)	0.0028(5)	0.0054(5)	-0.0002(5)
N2B	0.0193(5)	0.0230(6)	0.0230(6)	0.0004(4)	0.0068(4)	0.0009(4)
C1C	0.0211(6)	0.0211(6)	0.0219(6)	-0.0023(5)	0.0030(5)	-0.0016(5)
O1C	0.0213(5)	0.0235(5)	0.0308(5)	0.0019(4)	0.0087(4)	0.0020(4)

C2C	0.0239(6)	0.0280(7)	0.0299(7)	-0.0009(6)	0.0102(5)	-0.0005(5)
C3C	0.0305(7)	0.0286(7)	0.0294(7)	0.0022(6)	0.0112(6)	-0.0041(6)
C4C	0.0280(7)	0.0220(7)	0.0256(7)	-0.0012(5)	0.0010(5)	-0.0023(5)
C5C	0.0226(6)	0.0247(7)	0.0327(7)	-0.0033(6)	0.0062(5)	0.0007(5)
C6C	0.0216(6)	0.0242(7)	0.0296(7)	-0.0012(5)	0.0082(5)	-0.0035(5)
C7C	0.0330(7)	0.0228(7)	0.0308(8)	0.0013(6)	0.0004(6)	-0.0019(6)
C8C	0.0243(6)	0.0218(7)	0.0264(7)	0.0013(5)	0.0035(5)	0.0023(5)
N2C	0.0193(5)	0.0217(6)	0.0241(6)	0.0005(4)	0.0077(4)	0.0009(4)
C1D	0.0234(6)	0.0257(7)	0.0280(7)	-0.0034(5)	0.0079(5)	0.0014(5)
O1D	0.0234(5)	0.0297(6)	0.0393(6)	-0.0108(5)	0.0006(4)	0.0046(4)
C2D	0.0248(7)	0.0302(8)	0.0280(7)	-0.0025(6)	0.0034(5)	0.0032(5)
C3D	0.0299(7)	0.0320(8)	0.0290(7)	-0.0060(6)	0.0035(6)	-0.0017(6)
C4D	0.0308(7)	0.0266(7)	0.0286(7)	-0.0005(6)	0.0140(6)	-0.0005(5)
C5D	0.0275(7)	0.0285(8)	0.0385(8)	-0.0014(6)	0.0054(6)	0.0049(6)
C6D	0.0245(7)	0.0312(8)	0.0373(8)	-0.0072(6)	-0.0001(6)	0.0025(6)
C7D	0.0370(8)	0.0260(7)	0.0336(8)	-0.0025(6)	0.0176(6)	-0.0015(6)
C8D	0.0334(7)	0.0270(7)	0.0295(7)	-0.0043(6)	0.0149(6)	-0.0022(6)
N2D	0.0212(5)	0.0255(6)	0.0184(5)	-0.0009(4)	0.0056(4)	-0.0015(4)
N1E	0.0164(5)	0.0318(6)	0.0205(5)	-0.0004(5)	0.0050(4)	-0.0005(4)
C2E	0.0199(6)	0.0343(8)	0.0231(6)	0.0005(6)	0.0073(5)	-0.0005(5)
O2E	0.0209(5)	0.0812(9)	0.0212(5)	-0.0021(5)	0.0068(4)	-0.0023(5)
N3E	0.0167(5)	0.0314(6)	0.0231(6)	0.0006(5)	0.0059(4)	0.0003(4)
C4E	0.0190(6)	0.0222(6)	0.0239(6)	-0.0004(5)	0.0057(5)	0.0011(5)
O4E	0.0178(5)	0.0506(7)	0.0278(5)	-0.0037(5)	0.0033(4)	-0.0003(4)
C5E	0.0189(6)	0.0237(6)	0.0201(6)	-0.0011(5)	0.0051(5)	0.0022(5)
C6E	0.0200(6)	0.0180(6)	0.0231(6)	0.0001(5)	0.0066(5)	0.0012(4)
O6E	0.0200(5)	0.0347(6)	0.0248(5)	-0.0009(4)	0.0086(4)	0.0024(4)
C7E	0.0273(7)	0.0312(8)	0.0256(7)	0.0062(6)	0.0057(5)	0.0052(6)
C8E	0.0482(10)	0.0264(8)	0.0465(10)	0.0090(7)	0.0154(8)	0.0065(7)

C9E	0.0280(7)	0.0271(7)	0.0293(7)	-0.0069(6)	0.0041(6)	0.0014(5)
C10E	0.0462(10)	0.0233(8)	0.0489(10)	-0.0030(7)	0.0042(8)	0.0005(7)
N1F	0.0199(5)	0.0388(7)	0.0151(5)	-0.0004(5)	0.0054(4)	0.0046(5)
C2F	0.0188(6)	0.0284(7)	0.0193(6)	0.0010(5)	0.0058(5)	0.0041(5)
O2F	0.0195(5)	0.0600(7)	0.0186(5)	-0.0025(5)	0.0030(4)	0.0083(4)
N3F	0.0212(5)	0.0289(6)	0.0170(5)	-0.0003(4)	0.0065(4)	0.0009(4)
C4F	0.0227(6)	0.0278(7)	0.0184(6)	-0.0004(5)	0.0061(5)	-0.0023(5)
O4F	0.0318(6)	0.0662(8)	0.0177(5)	-0.0053(5)	0.0080(4)	-0.0044(5)
C5F	0.0195(6)	0.0295(7)	0.0173(6)	-0.0005(5)	0.0037(5)	-0.0012(5)
C6F	0.0212(6)	0.0280(7)	0.0189(6)	0.0005(5)	0.0051(5)	0.0006(5)
O6F	0.0213(5)	0.0551(7)	0.0256(5)	-0.0023(5)	0.0099(4)	0.0007(4)
C7F	0.0268(7)	0.0341(8)	0.0248(7)	0.0029(6)	0.0020(5)	0.0030(6)
C8F	0.0469(10)	0.0330(9)	0.0478(10)	0.0071(8)	0.0074(8)	0.0009(7)
C9F	0.0267(7)	0.0328(8)	0.0334(8)	-0.0079(6)	0.0089(6)	-0.0075(6)
C10F	0.0459(10)	0.0297(9)	0.0639(12)	0.0011(8)	0.0169(9)	-0.0052(7)
N1G	0.0198(5)	0.0344(6)	0.0148(5)	0.0002(4)	0.0048(4)	0.0048(4)
C2G	0.0191(6)	0.0230(6)	0.0193(6)	-0.0010(5)	0.0053(5)	0.0026(5)
O2G	0.0211(5)	0.0503(7)	0.0183(5)	-0.0010(4)	0.0037(4)	0.0098(4)
N3G	0.0207(5)	0.0285(6)	0.0170(5)	-0.0023(4)	0.0065(4)	-0.0020(4)
C4G	0.0229(6)	0.0356(8)	0.0172(6)	-0.0026(5)	0.0059(5)	-0.0059(5)
O4G	0.0299(6)	0.1033(11)	0.0164(5)	-0.0037(6)	0.0068(4)	-0.0061(6)
C5G	0.0196(6)	0.0285(7)	0.0176(6)	0.0013(5)	0.0034(5)	-0.0015(5)
C6G	0.0201(6)	0.0252(7)	0.0187(6)	0.0008(5)	0.0049(5)	0.0000(5)
O6G	0.0202(5)	0.0485(7)	0.0245(5)	0.0025(4)	0.0088(4)	0.0023(4)
C7G	0.0376(8)	0.0303(8)	0.0259(7)	0.0054(6)	0.0029(6)	0.0015(6)
C8G	0.0636(12)	0.0278(9)	0.0468(11)	0.0036(8)	0.0023(9)	-0.0062(8)
C9G	0.0219(6)	0.0327(8)	0.0250(7)	-0.0026(6)	0.0023(5)	-0.0046(5)
C10G	0.0410(9)	0.0302(8)	0.0417(9)	-0.0009(7)	0.0047(7)	-0.0086(7)
N1H	0.0160(5)	0.0314(6)	0.0210(5)	0.0006(5)	0.0055(4)	0.0008(4)

C2H	0.0189(6)	0.0263(7)	0.0234(6)	-0.0008(5)	0.0073(5)	-0.0009(5)
O2H	0.0214(5)	0.0552(7)	0.0214(5)	0.0034(5)	0.0063(4)	-0.0007(4)
N3H	0.0175(5)	0.0263(6)	0.0222(5)	0.0000(4)	0.0065(4)	0.0003(4)
C4H	0.0179(6)	0.0188(6)	0.0250(6)	-0.0020(5)	0.0054(5)	0.0001(4)
O4H	0.0171(4)	0.0387(6)	0.0273(5)	-0.0006(4)	0.0029(4)	0.0004(4)
C5H	0.0191(6)	0.0254(7)	0.0209(6)	0.0021(5)	0.0057(5)	0.0018(5)
C6H	0.0190(6)	0.0174(6)	0.0234(6)	-0.0004(5)	0.0066(5)	0.0006(4)
O6H	0.0201(4)	0.0333(5)	0.0254(5)	0.0006(4)	0.0099(4)	0.0023(4)
C7H	0.0274(7)	0.0315(8)	0.0415(9)	0.0140(7)	0.0114(6)	0.0060(6)
C8H	0.0481(10)	0.0241(8)	0.0715(13)	0.0038(8)	0.0296(9)	0.0004(7)
C9H	0.0260(7)	0.0412(9)	0.0221(7)	-0.0064(6)	0.0036(5)	0.0022(6)
C10H	0.0401(9)	0.0327(9)	0.0451(10)	-0.0150(7)	0.0112(7)	-0.0023(7)
C11	0.0331(8)	0.0361(9)	0.0547(11)	0.0103(8)	0.0080(8)	-0.0014(7)
Cl11	0.0598(12)	0.0324(7)	0.0420(10)	0.0002(5)	0.0113(8)	-0.0006(7)
Cl12	0.0399(13)	0.0564(11)	0.0517(14)	0.0231(11)	-0.0084(8)	-0.0184(7)
Cl13	0.0512(3)	0.0396(2)	0.0446(2)	-0.00324(18)	0.00756(19)	0.00298(18)
Cl14	0.104(5)	0.0395(13)	0.069(3)	-0.0033(17)	-0.012(2)	-0.010(2)
Cl15	0.085(4)	0.074(3)	0.095(4)	0.055(3)	-0.025(3)	-0.023(2)
C22	0.0366(8)	0.0352(9)	0.0373(9)	-0.0081(7)	0.0039(7)	-0.0032(7)
Cl21	0.0527(7)	0.0482(8)	0.0662(13)	-0.0112(7)	-0.0027(6)	0.0167(6)
Cl22	0.0415(9)	0.0293(8)	0.0554(11)	-0.0049(7)	-0.0010(8)	-0.0054(5)
Cl23	0.0599(13)	0.0738(14)	0.0449(8)	-0.0190(9)	0.0186(9)	-0.0202(7)
Cl24	0.0532(16)	0.0390(16)	0.139(7)	-0.034(3)	-0.014(3)	0.0054(11)
Cl25	0.087(4)	0.041(2)	0.062(2)	-0.0123(14)	0.027(2)	-0.0163(17)
Cl26	0.127(5)	0.065(2)	0.072(2)	0.0044(19)	0.063(3)	-0.025(3)
C33	0.0365(9)	0.0376(9)	0.0439(10)	0.0014(7)	0.0064(7)	-0.0040(7)
Cl31	0.0506(16)	0.0271(15)	0.0533(15)	0.0012(14)	0.0112(12)	-0.0002(13)
Cl32	0.0514(3)	0.0452(3)	0.0437(2)	0.01060(19)	0.00272(19)	0.00174(19)
Cl33	0.0572(18)	0.0398(13)	0.0459(10)	-0.0104(8)	0.0095(10)	0.0046(10)

Cl34	0.0451(15)	0.052(2)	0.0542(16)	-0.0186(16)	0.0038(12)	0.0164(15)
Cl36	0.074(3)	0.0436(9)	0.0338(8)	-0.0050(6)	0.0015(12)	-0.0003(15)
C44	0.0343(8)	0.0443(10)	0.0387(9)	-0.0114(8)	0.0053(7)	0.0026(7)
Cl41	0.0485(11)	0.0392(6)	0.0589(9)	0.0017(6)	-0.0040(5)	-0.0099(4)
Cl42	0.0782(14)	0.0988(14)	0.0898(15)	-0.0206(11)	0.0578(13)	-0.0125(10)
Cl43	0.0395(5)	0.0448(6)	0.0867(19)	-0.0140(10)	0.0043(9)	0.0124(4)
Cl44	0.134(4)	0.0435(18)	0.073(3)	-0.0180(16)	0.008(2)	-0.0088(18)
Cl45	0.0527(18)	0.133(5)	0.0488(16)	0.0165(19)	0.0185(13)	0.010(2)
Cl46	0.0528(12)	0.0407(13)	0.074(3)	-0.0214(17)	0.0005(16)	0.0042(10)

Table S5 Bond lengths in (I) (Å).

C1A—O1A	1.3674(17)	C9E—C10E	1.521(2)
C1A—C2A	1.3915(19)	C9E—H9E1	0.9900
C1A—C6A	1.3924(19)	C9E—H9E2	0.9900
O1A—H1A	0.787(19)	C10E—H10E	0.975(9)
C2A—C3A	1.390(2)	C10E—H11E	0.977(9)
C2A—H2A	0.9500	C10E—H12E	0.974(9)
C3A—C4A	1.395(2)	N1F—C6F	1.3542(17)
C3A—H3A	0.9500	N1F—C2F	1.3881(16)
C4A—C5A	1.390(2)	N1F—H1F	0.883(9)
C4A—C7A	1.511(2)	C2F—O2F	1.2496(16)
C5A—C6A	1.386(2)	C2F—N3F	1.3343(16)
C5A—H5A	0.9500	N3F—C4F	1.3521(17)
C6A—H6A	0.9500	C4F—O4F	1.2306(16)
C7A—C8A	1.5231(19)	C4F—C5F	1.5369(18)
C7A—H7A1	0.9900	C5F—C6F	1.5183(18)
C7A—H7A2	0.9900	C5F—C7F	1.5431(19)
C8A—N2A	1.4874(18)	C5F—C9F	1.5462(19)

C8A—H8A1	0.9900	C6F—O6F	1.2235(16)
C8A—H8A2	0.9900	C7F—C8F	1.525(2)
N2A—H11A	0.905(9)	C7F—H7F1	0.9900
N2A—H12A	0.905(9)	C7F—H7F2	0.9900
N2A—H13A	0.909(9)	C8F—H81F	0.980(9)
C1B—O1B	1.3615(17)	C8F—H83F	0.979(9)
C1B—C6B	1.3887(19)	C8F—H82F	0.981(9)
C1B—C2B	1.3973(19)	C9F—C10F	1.521(2)
O1B—H1B	0.804(18)	C9F—H9F1	0.9900
C2B—C3B	1.390(2)	C9F—H9F2	0.9900
C2B—H2B	0.9500	C10F—H10F	0.983(9)
C3B—C4B	1.394(2)	C10F—H11F	0.977(9)
C3B—H3B	0.9500	C10F—H12F	0.981(9)
C4B—C5B	1.391(2)	N1G—C6G	1.3565(16)
C4B—C7B	1.514(2)	N1G—C2G	1.3889(16)
C5B—C6B	1.391(2)	N1G—H1G	0.885(9)
C5B—H5B	0.9500	C2G—O2G	1.2521(15)
C6B—H6B	0.9500	C2G—N3G	1.3299(16)
C7B—C8B	1.514(2)	N3G—C4G	1.3558(17)
C7B—H7B1	0.9900	C4G—O4G	1.2287(16)
C7B—H7B2	0.9900	C4G—C5G	1.5328(19)
C8B—N2B	1.4916(18)	C5G—C6G	1.5173(18)
C8B—H8B1	0.9900	C5G—C9G	1.5445(19)
C8B—H8B2	0.9900	C5G—C7G	1.547(2)
N2B—H11B	0.908(9)	C6G—O6G	1.2239(15)
N2B—H12B	0.916(9)	C7G—C8G	1.526(2)
N2B—H13B	0.909(9)	C7G—H7G1	0.9900
C1C—O1C	1.3631(16)	C7G—H7G2	0.9900
C1C—C2C	1.3939(19)	C8G—H83G	0.977(9)

C1C—C6C	1.3953(18)	C8G—H82G	0.976(9)
O1C—H1C	0.802(18)	C8G—H81G	0.974(9)
C2C—C3C	1.389(2)	C9G—C10G	1.520(2)
C2C—H2C	0.9500	C9G—H9G1	0.9900
C3C—C4C	1.394(2)	C9G—H9G2	0.9900
C3C—H3C	0.9500	C10G—H10G	0.981(9)
C4C—C5C	1.393(2)	C10G—H11G	0.979(9)
C4C—C7C	1.508(2)	C10G—H12G	0.985(9)
C5C—C6C	1.389(2)	N1H—C6H	1.3532(17)
C5C—H5C	0.9500	N1H—C2H	1.4031(16)
C6C—H6C	0.9500	N1H—H1H	0.875(9)
C7C—C8C	1.5190(19)	C2H—O2H	1.2383(16)
C7C—H7C1	0.9900	C2H—N3H	1.3463(17)
C7C—H7C2	0.9900	N3H—C4H	1.3543(17)
C8C—N2C	1.4871(17)	C4H—O4H	1.2354(15)
C8C—H8C1	0.9900	C4H—C5H	1.5431(18)
C8C—H8C2	0.9900	C5H—C6H	1.5139(18)
N2C—H11C	0.907(9)	C5H—C9H	1.5427(19)
N2C—H12C	0.911(9)	C5H—C7H	1.549(2)
N2C—H13C	0.912(9)	C6H—O6H	1.2339(15)
C1D—O1D	1.3705(17)	C7H—C8H	1.520(3)
C1D—C6D	1.389(2)	C7H—H7H1	0.9900
C1D—C2D	1.3906(19)	C7H—H7H2	0.9900
O1D—H1D	0.812(19)	C8H—H83H	0.982(9)
C2D—C3D	1.390(2)	C8H—H81H	0.984(9)
C2D—H2D	0.9500	C8H—H82H	0.980(9)
C3D—C4D	1.396(2)	C9H—C10H	1.522(2)
C3D—H3D	0.9500	C9H—H9H1	0.9900
C4D—C5D	1.390(2)	C9H—H9H2	0.9900

C4D—C7D	1.511(2)	C10H—H10H	0.985(9)
C5D—C6D	1.386(2)	C10H—H11H	0.986(9)
C5D—H5D	0.9500	C10H—H12H	0.982(9)
C6D—H6D	0.9500	C11—Cl11	1.736(4)
C7D—C8D	1.521(2)	C11—Cl15	1.742(7)
C7D—H7D1	0.9900	C11—Cl13	1.7604(19)
C7D—H7D2	0.9900	C11—Cl12	1.772(4)
C8D—N2D	1.4904(18)	C11—Cl14	1.781(11)
C8D—H8D1	0.9900	C11—H11	0.92(2)
C8D—H8D2	0.9900	C22—Cl26	1.722(6)
N2D—H11D	0.903(9)	C22—Cl25	1.727(8)
N2D—H12D	0.900(9)	C22—Cl21	1.751(4)
N2D—H13D	0.905(9)	C22—Cl24	1.762(8)
N1E—C6E	1.3531(17)	C22—Cl23	1.769(4)
N1E—C2E	1.4009(17)	C22—Cl22	1.770(4)
N1E—H1E	0.876(9)	C22—H22	0.93(2)
C2E—O2E	1.2407(17)	C33—Cl33	1.700(6)
C2E—N3E	1.3438(17)	C33—Cl34	1.742(5)
N3E—C4E	1.3486(17)	C33—Cl32	1.7562(18)
C4E—O4E	1.2339(16)	C33—Cl31	1.776(5)
C4E—C5E	1.5393(18)	C33—Cl36	1.818(9)
C5E—C6E	1.5168(18)	C33—H33	0.96(2)
C5E—C7E	1.5429(19)	C44—Cl44	1.657(8)
C5E—C9E	1.5517(19)	C44—Cl42	1.697(4)
C6E—O6E	1.2317(15)	C44—Cl43	1.724(3)
C7E—C8E	1.524(2)	C44—Cl41	1.795(3)
C7E—H7E1	0.9900	C44—Cl46	1.824(7)
C7E—H7E2	0.9900	C44—Cl45	1.848(8)
C8E—H81E	0.981(9)	C44—H44	0.97(2)

C8E—H82E	0.985(9)	Cl43—Cl46	0.506(7)
C8E—H83E	0.982(9)		

Table S6 Valence angles in (I) (°).

O1A—C1A—C2A	122.37(12)	C6F N1F H1F	116.6(11)
O1A—C1A—C6A	117.80(12)	C2F—N1F—H1F	121.72(12)
C2A—C1A—C6A	119.83(13)	O2F—C2F—N3F	116.14(11)
C1A—O1A—H1A	112.5(14)	O2F—C2F—N1F	122.14(11)
C3A—C2A—C1A	119.49(13)	N3F—C2F—N1F	119.78(11)
C3A—C2A—H2A	120.3	C2F—N3F—C4F	119.35(12)
C1A—C2A—H2A	120.3	O4F—C4F—N3F	117.79(12)
C2A—C3A—C4A	121.54(13)	O4F—C4F—C5F	122.84(11)
C2A—C3A—H3A	119.2	N3F—C4F—C5F	113.04(11)
C4A—C3A—H3A	119.2	C6F—C5F—C4F	108.38(11)
C5A—C4A—C3A	117.85(13)	C6F—C5F—C7F	110.14(11)
C5A—C4A—C7A	121.28(13)	C4F—C5F—C7F	107.62(11)
C3A—C4A—C7A	120.84(13)	C6F—C5F—C9F	108.89(11)
C6A—C5A—C4A	121.59(13)	C4F—C5F—C9F	108.65(11)
C6A—C5A—H5A	119.2	C7F—C5F—C9F	120.90(12)
C4A—C5A—H5A	119.2	O6F—C6F—N1F	122.01(12)
C5A—C6A—C1A	119.70(13)	O6F—C6F—C5F	117.09(11)
C5A—C6A—H6A	120.2	N1F—C6F—C5F	114.31(12)
C1A—C6A—H6A	120.2	C8F—C7F—C5F	108.7
C4A—C7A—C8A	110.47(11)	C8F—C7F—H7F1	108.7
C4A—C7A—H7A1	109.6	C5F—C7F—H7F1	108.7
C8A—C7A—H7A1	109.6	C8F—C7F—H7F2	108.7
C4A—C7A—H7A2	109.6	C5F—C7F—H7F2	107.6
C8A—C7A—H7A2	109.6	H7F1—C7F—H7F2	109.7(14)
H7A—C7A—H7A2	108.1	C7F—C8F—H81F	112.2(13)

N2A—C8A—C7A	112.32(11)	C7F—C8F—H83F	110.9(18)
N2A—C8A—H8A1	109.1	H81F—C8F—H83F	110.0(13)
C7A—C8A—H8A1	109.1	C7F—C8F—H82F	107.2(18)
N2A—C8A—H8A2	109.1	H81F—C8F—H82F	106.7(19)
C7A—C8A—H8A2	109.1	H83F—C8F—H82F	113.99(13)
H8A1—C8A—H8A2	107.9	C10F—C9F—C5F	108.8
C8A—N2A—H11A	110.2(11)	C10F—C9F—H9F1	108.8
C8A—N2A—H12A	107.5(11)	C5F—C9F—H9F1	108.8
H11A—N2A—H12A	114.3(15)	C10F—C9F—H9F2	108.8
C8A—N2A—H13A	105.9(11)	C5F—C9F—H9F2	107.6
H11A—N2A—H13A	108.4(15)	H9F1—C9F—H9F2	111.0(14)
H12A—N2A—H13A	110.2(15)	C9F—C10F—H10F	111.2(14)
O1B—C1B—C6B	117.35(12)	C9F—C10F—H11F	109.8(19)
O1B—C1B—C2B	123.26(12)	H10F—C10F—H11F	113.0(13)
C6B—C1B—C2B	119.40(13)	C9F—C10F—H12F	106.2(19)
C1B—O1B—H1B	111.3(12)	H10F—C10F—H12F	105.3(19)
C3B—C2B—C1B	119.52(14)	H11F—C10F—H12F	124.87(11)
C3B—C2B—H2B	120.2	C6G—N1G—C2G	118.7(11)
C1B—C2B—H2B	120.2	C6G—N1G—H1G	116.4(11)
C2B—C3B—C4B	121.80(14)	C2G—N1G—H1G	121.45(11)
C2B—C3B—H3B	119.1	O2G—C2G—N3G	116.20(11)
C4B—C3B—H3B	119.1	O2G—C2G—N1G	122.34(11)
C5B—C4B—C3B	117.75(14)	N3G—C2G—N1G	119.60(11)
C5B—C4B—C7B	121.52(14)	C2G—N3G—C4G	118.99(12)
C3B—C4B—C7B	120.72(14)	O4G—C4G—N3G	118.07(12)
C4B—C5B—C6B	121.32(14)	O4G—C4G—C5G	122.93(11)
C4B—C5B—H5B	119.3	N3G—C4G—C5G	113.03(11)
C6B—C5B—H5B	119.3	C6G—C5G—C4G	108.23(11)
C1B—C6B—C5B	120.20(13)	C6G—C5G—C9G	108.95(11)

C1B—C6B—H6B	119.9	C4G—C5G—C9G	108.46(11)
C5B—C6B—H6B	119.9	C6G—C5G—C7G	109.12(11)
C4B—C7B—C8B	110.67(12)	C4G—C5G—C7G	108.99(11)
C4B—C7B H7B1	109.5	C9G—C5G—C7G	120.79(12)
C8B—C7B—H7B1	109.5	O6G—C6G—N1G	122.15(12)
C4B—C7B—H7B2	109.5	O6G—C6G—C5G	117.06(11)
C8B—C7B—H7B2	109.5	N1G—C6G—C5G	114.12(13)
H7B1—C7B—H7B2	108.1	C8G—C7G—C5G	108.7
N2B—C8B—C7B	110.42(11)	C8G—C7G—H7G1	108.7
N2B—C8B—H8B1	109.6	C5G—C7G—H7G1	108.7
C7B—C8B—H8B1	109.6	C8G—C7G—H7G2	108.7
N2B—C8B—H8B2	109.6	C5G—C7G—H7G2	107.6
C7B—C8B—H8B2	109.6	H7G1—C7G—H7G2	110.1(14)
H8B1—C8B—H8B2	108.1	C7G—C8G—H83G	114.6(14)
C8B—N2B—H11B	103.0(11)	C7G—C8G—H82G	107(2)
C8B—N2B—H12B	110.4(11)	H83G—C8G—H82G	110.7(14)
H11B—N2B—H12B	111.4(15)	C7G—C8G—H81G	108.8(19)
C8B—N2B—H13B	111.7(11)	H83G—C8G—H81G	105.3(19)
H11B—N2B—H13B	110.4(15)	H82G—C8G—H81G	113.97(12)
H12B—N2B—H13B	109.7(15)	C10G—C9G—C5G	108.8
O1C—C1C—C2C	122.87(12)	C10G—C9G—H9G1	108.8
O1C—C1C—C6C	117.72(12)	C5G—C9G—H9G1	108.8
C2C—C1C—C6C	119.41(13)	C10G—C9G—H9G2	108.8
C1C—O1C—H1C	109.8(13) .	C5G—C9G—H9G2	107.7
C3C—C2C—C1C	119.88(13)	H9G1—C9G—H9G2	109.3(12)
C3C—C2C—H2C	120.1	C9G—C10G—H10G	110.5(13)
C1C—C2C—H2C	120.1	C9G—C10G—H11G	108.2(17)
C2C—C3C—C4C	121.56(13)	H10G—C10G—H11G	110.1(13)
C2C—C3C—H3C	119.2	C9G—C10G—H12G	108.9(17)

C4C—C3C—H3C	119.2	H10G—C10G—H12G	109.9(17)
C5C—C4C—C3C	117.73(13)	H11G—C10G—H12G	124.62(11)
C5C—C4C—C7C	121.04(13)	C6H—N1H—C2H	120.9(11)
C3C—C4C—C7C	121.17(13)	C6H—N1H—H1H	114.4(11)
C6C—C5C—C4C	121.64(13)	C2H—N1H—H1H	121.63(12)
C6C—C5C—H5C	119.2	O2H—C2H—N3H	116.81(12)
C4C—C5C—H5C	119.2	O2H—C2H—N1H	121.57(12)
C5C—C6C—C1C	119.79(13)	N3H—C2H—N1H	120.51(11)
C5C—C6C—H6C	120.1	C2H—N3H—C4H	121.31(12)
C1C—C6C—H6C	120.1	O4H—C4H—N3H	116.78(12)
C4C—C7C—C8C	110.71(12)	O4H—C4H—C5H	121.91(11)
C4C—C7C—H7C1	109.5	N3H—C4H—C5H	108.78(11)
C8C—C7C—H7C1	109.5	C6H—C5H—C9H	113.65(11)
C4C—C7C—H7C2	109.5	C6H—C5H—C4H	108.67(11)
C8C—C7C—H7C2	109.5	C9H—C5H—C4H	107.62(11)
H7C1—C7C—H7C2	108.1	C6H—C5H—C7H	108.95(12)
N2C—C8C—C7C	110.81(11)	C9H—C5H—C7H	109.08(11)
N2C—C8C—H8C1	109.5	C4H—C5H—C7H	121.25(12)
C7C—C8C—H8C1	109.5	O6H—C6H—N1H	121.23(12)
N2C—C8C—H8C2	109.5	O6H—C6H—C5H	117.51(11)
C7C—C8C—H8C2	109.5	N1H—C6H—C5H	114.56(13)
H8C1—C8C—H8C2	108.1	C8H—C7H—C5H	108.6
C8C—N2C—H11C	103.4(11)	C8H—C7H—H7H1	108.6
C8C—N2C—H12C	109.2(11)	C5H—C7H—H7H1	108.6
H11C—N2C—H12C	110.6(15)	C8H—C7H—H7H2	108.6
C8C—N2C—H13C	108.9(11) .	C5H—C7H—H7H2	107.6
H11C—N2C—H13C	112.1(15)	H7H1—C7H—H7H2	111.5(14)
H12C—N2C—H13C	112.1(15)	C7H—C8H—H83H	113.5(13)
O1D—C1D—C6D	117.86(13)	C7H—C8H—H81H	105.6(19)

O1D—C1D—C2D	122.28(13)	H83H—C8H—H81H	113.9(13)
C6D—C1D—C2D	119.86(13)	C7H—C8H—H82H	108.1(18)
C1D—O1D—H1D	112.1(13)	H83H—C8H—H82H	103.6(18)
C3D—C2D—C1D	119.40(13)	H81H—C8H—H82H	114.22(12)
C3D—C2D—H2D	120.3	C10H—C9H—C5H	108.7
C1D—C2D—H2D	120.3	C10H—C9H—H9H1	108.7
C2D—C3D—C4D	121.59(13)	C5H—C9H—H9H1	108.7
C2D—C3D—H3D	119.2	C10H—C9H—H9H2	108.7
C4D—C3D—H3D	119.2	C5H—C9H—H9H2	107.6
C5D—C4D—C3D	117.73(13)	H9H1—C9H—H9H2	112.1(13)
C5D—C4D—C7D	121.11(14)	C9H—C10H—H10H	111.3(13)
C3D—C4D—C7D	121.05(13)	C9H—C10H—H11H	109.4(17)
C6D—C5D—C4D	121.52(14)	H10H—C10H—H11H	110.7(13)
C6D—C5D—H5D	119.2	C9H—C10H—H12H	105.8(17)
C4D—C5D—H5D	119.2	H10H—C10H—H12H	107.2(17)
C5D—C6D—C1D	119.87(14)	H11H—C10H—H12H	116.0(5)
C5D—C6D—H6D	120.1	Cl11—C11—Cl15	113.08(17)
C1D—C6D—H6D	120.1	Cl11—C11—Cl13	107.8(3)
C4D—C7D—C8D	109.64(12)	Cl15—C11—Cl13	110.8(2)
C4D—C7D—H7D1	109.7	Cl11—C11 Cl12	5.5(5)
C8D—C7D—H7D1	109.7	Cl15—C11—Cl12	109.72(13)
C4D—C7D—H7D2	109.7	Cl13—C11—Cl12	10.9(9)
C8D—C7D—H7D2	109.7	Cl11—C11—Cl14	110.3(4)
H7D1—C7D—H7D2	108.2	Cl15—C11—Cl14	108.1(5)
N2D—C8D—C7D	113.03(11)	Cl13—C11—Cl14	104.9(5)
N2D—C8D—H8D1	109.0	Cl12—C11—Cl14	102.4(13)
C7D—C8D—H8D1	109.0	Cl11—C11—H11	106.6(13)
N2D—C8D—H8D2	109.0	Cl15—C11—H11	110.6(12)
C7D—C8D—H8D2	109.0	Cl13—C11—H11	110.1(12)

H8D1—C8D—H8D2	107.8	Cl12—C11—H11	113.3(16)
C8D—N2D—H11D	108.0(11)	Cl14—C11—H11	108.9(4)
C8D—N2D—H12D	107.2(11)	Cl26—C22—Cl25	107.4(6)
H11D—N2D—H12D	108.7(15)	Cl26—C22—Cl21	113.1(3)
C8D—N2D—H13D	111.5(11)	Cl25—C22—Cl21	94.5(13)
H11D—N2D—H13D	106.8(15)	Cl26—C22—Cl24	113.2(3)
H12D—N2D—H13D	114.4(16)	Cl25—C22—Cl24	14.4(8)
C6E—N1E—C2E	124.65(11)	Cl21—C22—Cl24	10.1(6)
C6E—N1E—H1E	122.7(11)	Cl26—C22—Cl23	105.8(4)
C2E—N1E—H1E	112.6(11)	Cl25—C22—Cl23	117.1(2)
O2E—C2E—N3E	121.74(12)	Cl21—C22—Cl23	104.4(8)
O2E—C2E—N1E	116.83(12)	Cl24—C22—Cl23	115.1(3)
N3E—C2E—N1E	121.43(12)	Cl26—C22—Cl22	6.1(5)
C2E—N3E—C4E	120.75(11)	Cl25—C22—Cl22	109.69(19)
O4E—C4E—N3E	121.33(12)	Cl21—C22—Cl22	111.3(2)
O4E—C4E—C5E	116.60(12)	Cl24—C22—Cl22	111.9(2)
N3E—C4E—C5E	122.06(11)	Cl23—C22—Cl22	111.9(13)
C6E—C5E—C4E	113.49(11)	Cl26—C22—H22	110.5(13)
C6E—C5E—C7E	109.00(11)	Cl25—C22—H22	104.9(12).
C4E—C5E—C7E	109.69(11)	Cl21—C22—H22	116.6(14)
C6E—C5E—C9E	107.59(10)	Cl24—C22—H22	105.1(12)
C4E—C5E—C9E	108.16(11)	Cl23—C22—H22	107.4(12)
C7E—C5E—C9E	108.79(11)	Cl22—C22—H22	114.3(3)
O6E—C6E—N1E	121.30(12)	Cl33—C33—Cl34	113.7(2)
O6E—C6E—C5E	121.16(12)	Cl33—C33—Cl32	110.0(2)
N1E—C6E—C5E	117.54(11)	Cl34—C33—Cl32	110.6(3)
C8E—C7E—C5E	114.38(12)	Cl33—C33—Cl31	4.2(4)
C8E—C7E—H7E1	108.7	Cl34—C33—Cl31	110.9(2)
C5E—C7E—H7E1	108.7	Cl32—C33—Cl31	11.7(2)

C8E—C7E—H7E2	108.7	Cl33—C33—Cl36	109.6(3).
C5E—C7E—H7E2	108.7	Cl34—C33—Cl36	107.4(3)
H7E1—C7E—H7E2	107.6	Cl32—C33—Cl36	105.6(3)
C7E—C8E—H81E	110.1(13)	Cl31—C33—Cl36	101.7(12)
C7E—C8E—H82E	111.1(13)	Cl33—C33—H33	106.9(12)
H81E—C8E—H82E	110.1(18)	Cl34—C33—H33	109.5(12)
C7E—C8E—H83E	110.1(13)	Cl32—C33—H33	109.9(12)
H81E—C8E—H83E	109.4(17)	Cl31—C33—H33	113.4(12)
H82E—C8E—H83E	105.9(17)	Cl36—C33—H33	100.2(4)
C10E—C9E—C5E	114.14(12)	Cl44—C44—Cl42	112.4(3)
C10E—C9E—H9E1	108.7	Cl44—C44—Cl43	116.8(3)
C5E—C9E—H9E1	108.7	Cl42—C44—Cl43	10.2(5)
C10E—C9E—H9E2	108.7	Cl44—C44—Cl41	109.9(2)
C5E—C9E—H9E2	108.7	Cl42—C44—Cl41	109.02(16)
H9E1—C9E—H9E2	107.6	Cl43—C44—Cl41	112.7(3)
C9E—C10E—H10E	112.5(13)	Cl44—C44—Cl46	101.6(4)
C9E—C10E—H11E	112.5(13)	Cl42—C44—Cl46	16.09(19)
H10E—C10E—H11E	105.7(18)	Cl43—C44—Cl46	112.3(2)
C9E—C10E—H12E	109.7(13)	Cl41—C44—Cl46	110.0(4)
H10E—C10E—H12E	105.9(18)	Cl44—C44—Cl45	9.9(4)
H11E—C10E—H12E	110.3(18)	Cl42—C44—Cl45	111.8(4)
C6F—N1F—C2F	125.07(11)	Cl43—C44—Cl45	119.7(4)
C6F—N1F—H1F	118.2(11)	Cl41—C44—Cl45	97.7(5)

Table S7 Torsion angles in (I) (°).

O1A—C1A—C2A—C3A	179.65(13)	C2F—N3F—C4F—C5F	-1.4(2)
C6A—C1A—C2A—C3A	-0.7(2)	O4F—C4F—C5F—C6F	-179.49(13)
C1A—C2A—C3A—C4A	0.0(2)	N3F—C4F—C5F—C6F	1.62(19)
C2A—C3A—C4A—C5A	0.7(2)	O4F—C4F—C5F—C7F	-58.09(17)

C2A—C3A—C4A—C7A	-177.23(14)	N3F—C4F—C5F—C7F	123.02(14)
C3A—C4A—C5A—C6A	-0.8(2)	O4F—C4F—C5F—C9F	60.96(17)
C7A—C4A—C5A—C6A	177.17(14)	N3F—C4F—C5F—C9F	-117.93(14)
C4A—C5A—C6A—C1A	0.1(2)	C2F—N1F—C6F—O6F	178.39(14)
O1A—C1A—C6A—C5A	-179.68(13)	C2F—N1F—C6F—C5F	-1.1(2)
C2A—C1A—C6A—C5A	0.6(2)	C4F—C5F—C6F—O6F	-179.87(13)
C5A—C4A—C7A—C8A	-100.10(16)	C7F—C5F—C6F—O6F	57.74(17)
C3A—C4A—C7A—C8A	77.77(18)	C9F—C5F—C6F—O6F	-59.59(17)
C4A—C7A—C8A—N2A	-179.25(12)	C4F—C5F—C6F—N1F	-0.38(18)
O1B—C1B—C2B—C3B	-178.68(13)	C7F—C5F—C6F—N1F	-122.76(13)
C6B—C1B—C2B—C3B	0.7(2)	C9F—C5F—C6F—N1F	119.90(13)
C1B—C2B—C3B—C4B	0.1(2)	C6F—C5F—C7F—C8F	60.95(16)
C2B—C3B—C4B—C5B	-0.9(2)	C4F—C5F—C7F—C8F	-63.18(16)
C2B—C3B—C4B—C7B	-179.56(14)	C9F—C5F—C7F—C8F	177.62(13)
C3B—C4B—C5B—C6B	1.0(2)	C6F—C5F—C9F—C10F	-62.62(16)
C7B—C4B—C5B—C6B	179.66(14)	C4F—C5F—C9F—C10F	60.24(16)
O1B—C1B—C6B—C5B	178.83(13)	C7F—C5F—C9F—C10F	-179.78(13)
C2B—C1B—C6B—C5B	-0.5(2)	C6G—N1G—C2G—O2G	-178.14(13)
C4B—C5B—C6B—C1B	-0.3(2)	C6G—N1G—C2G—N3G	2.0(2)
C5B—C4B—C7B—C8B	-97.25(17)	O2G—C2G—N3G—C4G	177.48(13)
C3B—C4B—C7B—C8B	81.39(18)	N1G—C2G—N3G—C4G	-2.7(2)
C4B—C7B—C8B—N2B	-172.05(12)	C2G—N3G—C4G—O4G	-179.36(14)
O1C—C1C—C2C—C3C	-179.55(13)	C2G—N3G—C4G—C5G	-0.4(2)
C6C—C1C—C2C—C3C	0.6(2)	O4G—C4G—C5G—C6G	-177.27(14)
C1C—C2C—C3C—C4C	-0.2(2)	N3G—C4G—C5G—C6G	3.77(19)
C2C—C3C—C4C—C5C	0.0(2)	O4G—C4G—C5G—C9G	-56.92(18)
C2C—C3C—C4C—C7C	177.28(13)	N3G—C4G—C5G—C9G	124.11(14)
C3C—C4C—C5C—C6C	-0.2(2)	O4G—C4G—C5G—C7G	61.97(18)
C7C—C4C—C5C—C6C	-177.50(13)	N3G—C4G—C5G—C7G	-117.00(14)

C4C—C5C—C6C—C1C	0.6(2)	C2G—N1G—C6G—O6G	-178.77(13)
O1C—C1C—C6C—C5C	179.33(12)	C2G—N1G—C6G—C5G	1.8(2)
C2C—C1C—C6C—C5C	-0.8(2). .	C4G—C5G—C6G—O6G	176.32(13)
C5C—C4C—C7C—C8C	94.81(16)	C9G—C5G—C6G—O6G	55.57(17)
C3C—C4C—C7C—C8C	-82.40(17)	C7G—C5G—C6G—O6G	-62.54(17)
C4C—C7C—C8C—N2C	179.55(12)	C4G—C5G—C6G—N1G	-4.23(17)
O1D—C1D—C2D—C3D	-178.96(14)	C9G—C5G—C6G—N1G	-124.98(13)
C6D—C1D—C2D—C3D	1.7(2)	C7G—C5G—C6G—N1G	116.91(13)
C1D—C2D—C3D—C4D	-0.5(2)	C6G—C5G—C7G—C8G	-60.26(17)
C2D—C3D—C4D—C5D	-0.9(2)	C4G—C5G—C7G—C8G	63.26(17)
C2D—C3D—C4D—C7D	175.41(14)	C9G—C5G—C7G—C8G	-177.88(14)
C3D—C4D—C5D—C6D	1.0(2)	C6G—C5G—C9G—C10G	61.31(16)
C7D—C4D—C5D—C6D	-175.28(14)	C4G—C5G—C9G—C10G	-61.95(16)
C4D—C5D—C6D—C1D	0.2(2)	C7G—C5G—C9G—C10G	179.09(13)
O1D—C1D—C6D—C5D	179.04(14)	C6H—N1H—C2H—O2H	179.33(13)
C2D—C1D—C6D—C5D	-1.6(2)	C6H—N1H—C2H—N3H	-0.3(2)
C5D—C4D—C7D—C8D	92.05(17)	O2H—C2H—N3H—C4H	178.00(13)
C3D—C4D—C7D—C8D	-84.15(17)	N1H—C2H—N3H—C4H	-2.4(2)
C4D—C7D—C8D—N2D	-177.61(12)	C2H—N3H—C4H—O4H	-178.52(13)
C6E—N1E—C2E—O2E	-179.23(14)	C2H—N3H—C4H—C5H	0.61(19)
C6E—N1E—C2E—N3E	0.9(2)	O4H—C4H—C5H—C6H	-177.53(12)
O2E—C2E—N3E—C4E	-178.89(14)	N3H—C4H—C5H—C6H	3.31(17)
N1E—C2E—N3E—C4E	1.0(2)	O4H—C4H—C5H—C9H	-56.26(15)
C2E—N3E—C4E—O4E	178.34(13)	N3H—C4H—C5H—C9H	124.57(13)
C2E—N3E—C4E—C5E	-2.9(2)	O4H—C4H—C5H—C7H	62.40(16)
O4E—C4E—C5E—C6E	-178.23(12)	N3H—C4H—C5H—C7H	-116.77(14)
N3E—C4E—C5E—C6E	2.99(18)	C2H—N1H—C6H—O6H	-176.41(12)
O4E—C4E—C5E—C7E	-56.06(16)	C2H—N1H—C6H—C5H	4.45(19)
N3E—C4E—C5E—C7E	125.17(13)	C9H—C5H—C6H—O6H	54.09(16)

O4E—C4E—C5E—C9E	62.46(15)	C4H—C5H—C6H—O6H	175.30(12)
N3E—C4E—C5E—C9E	-116.32(14)	C7H—C5H—C6H—O6H	-63.81(16)
C2E—N1E—C6E—O6E	178.69(13)	C9H—C5H—C6H—N1H	-126.77(13)
C2E—N1E—C6E—C5E	-0.63(19)	C4H—C5H—C6H—N1H	-5.57(17)
C4E—C5E—C6E—O6E	179.51(12)	C7H—C5H—C6H—N1H	115.33(13)
C7E—C5E—C6E—O6E	56.95(16)	C6H—C5H—C7H—C8H	-61.17(16)
C9E—C5E—C6E—O6E	-60.87(16)	C9H—C5H—C7H—C8H	-178.97(13)
C4E—C5E—C6E—N1E	-1.17(17)	C4H—C5H—C7H—C8H	62.55(16)
C7E—C5E—C6E—N1E	-123.74(13)	C6H—C5H—C9H—C10H	62.66(15)
C9E—C5E—C6E—N1E	118.45(13)	C4H—C5H—C9H—C10H	-61.55(15)
C6E—C5E—C7E—C8E	66.11(15)	C7H—C5H—C9H—C10H	179.72(12)
C4E—C5E—C7E—C8E	-58.71(16)	Cl44—C44—Cl43—Cl46	94.3(10)
C9E—C5E—C7E—C8E	-176.83(12)	Cl42—C44—Cl43—Cl46	-20.6(11)
C6E—C5E—C9E—C10E	-61.54(16)	Cl41—C44—Cl43—Cl46	104.7(10)
C4E—C5E—C9E—C10E	61.42(15)	Cl45—C44—Cl43—Cl46	-30.0(10)
C7E—C5E—C9E—C10E	-179.49(13)	Cl44—C44—Cl46—Cl43	-92.4(10)
C6F—N1F—C2F—O2F	-178.71(13)	Cl42—C44—Cl46—Cl43	161.3(10)
C6F—N1F—C2F—N3F	1.5(2)	Cl41—C44—Cl46—Cl43	-81.3(10)
O2F—C2F—N3F—C4F	-179.93(13)	Cl45—C44—Cl46—Cl43	152.1(10)
N1F—C2F—N3F—C4F	-0.2(2)		
C2F—N3F—C4F—O4F	179.77(14)		

S2. Tyraminium 5,5-diethylbarbiturate (II)

Computing details:

Data collection: *CrysAlisPro 1.171.38.34a* (Rigaku OD, 2015); cell refinement: *CrysAlisPro 1.171.38.34a* (Rigaku OD, 2015), data reduction: *CrysAlisPro 1.171.38.34a* (Rigaku OD, 2015); program(s) used to solve structure: *SIR-92 (ALTOMARE et al., 1994)*; program(s) used to refine structure: *SHELXL-2018/3* (Sheldrick, 2015) in WinGX (Farrugia, 2012); molecular graphics: *ORTEP-3* (Farrugia, 1997) and Mercury 3.10.2 (Macrae *et al*., 2008); software used to prepare material for publication: SHELXL-2018/3 (Sheldrick, 2015).

Optical Indicatrix of (II)

Optical character and optical activity of (II) single crystals were determined using Zeiss Axio Scope.A1 polarizing microscope. Conoscopic image (Figure S2a) demonstrates uniaxial interference figure of (II) crystal approximately along [001]. Figure S2b, c and d present reactions with accessory plates: gypsum, mica and quartz wedge, respectively. Characteristic blue hue in negative quadrants (Figure S2b) and black dots in positive ones (Figure S2c) definitely proved the negative optical character of (II) crystals.

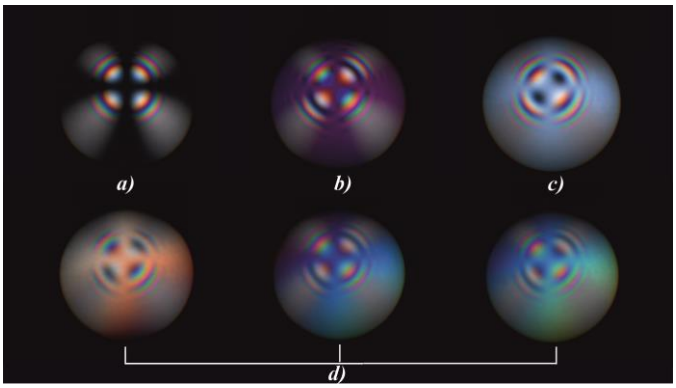

Figure S2 a) Conoscopic image of (II) crystal oriented almost along to the optical axis; the reaction of the crystal with the gypsum plate, the mica plate and the quartz wedge (b, c and d, respectively) showing uniaxial interference figures and negative optical character of (II).

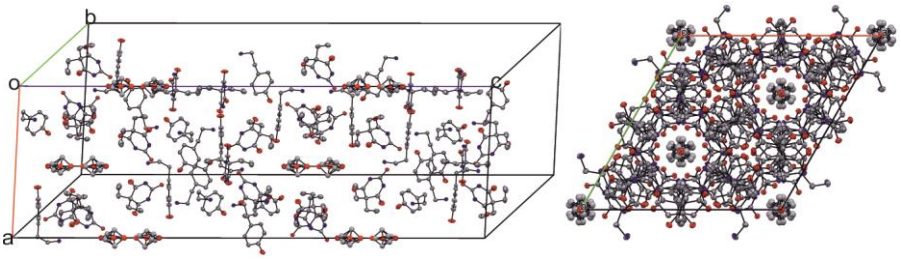

Figure S3 Packing of structural components in (II) with disordered solvent molecules located in cavities (left – general view, right – projection along [001]).

Table S8 Hydrogen-bond geometry (Å,°) for (II).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*B*—H1*B*···O6*A*^{ii}	0.87 (2)	1.83 (2)	2.696 (1)	178 (2)
N2*B*—H22···O2*A*^{i}	0.91 (1)	1.93 (1)	2.835 (1)	179 (1)

N2*B*—H21···N3*A*^{iii}	0.92 (1)	1.96 (1)	2.864 (1)	169 (1)
N1*A*—H1*A*···O2*A*^{i}	0.88 (1)	2.00 (1)	2.866 (1)	169 (1)
N2*B*—H23···O4*A*^{iv}	0.90 (1)	2.01 (1)	2.784 (1)	143 (1)
C8*B*—H8*B*1···O6*A*^{iii}	0.99	2.44	3.237 (1)	137
C2*B*—H2*B*···O6*A*^{ii}	0.95	2.48	3.180 (1)	131

Symmetry codes: (i) −*x*+*y*+2, −*x*+1, *z*; (ii) −*x*+4/3, −*x*+*y*+2/3, −*z*+1/6; (iii) *y*+4/3, *x*−1/3, −*z*+1/6; (iv) *x*−*y*+1/3, −*y*+2/3, −*z*+1/6.

Table S9 Hydrogen-bond geometry (Å,°) for (II).

C-H···π	D-H (Å)	H···A (Å)	D-A (Å)	D-H-A (°)
C7B-H7B1···Cg(C1B-^C6B)	0.98	2.51	3.434	156
C10A-H10B··· Cg(C1B-^C6B)	0.98	3.28	4.095	141

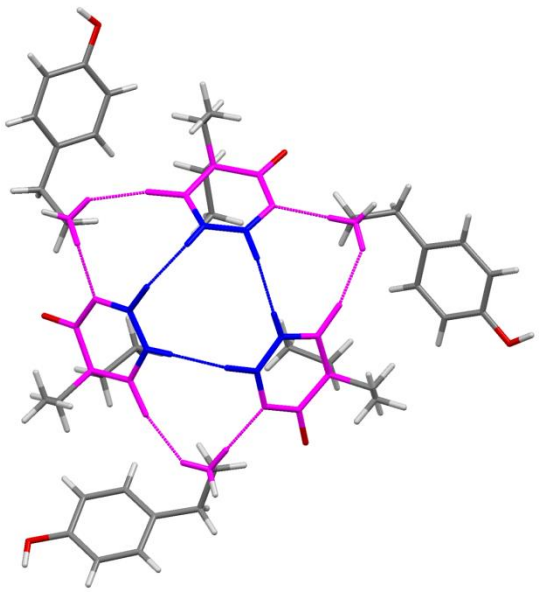

Figure S4 $R_3^3(12)$ and $R_6^6(24)$ ring motifs in (II).

Table S10 Fractional atomic coordinates and equivalent isotropic displacement parameters of (II) (Å^2).

	x	y	z	U_{iso}*/U_{eq}
N1A	0.92886(6)	0.09772(6)	0.08943(2)	0.0242(2)
H1A	0.9782(7)	0.1084(9)	0.0829(2)	0.029*
C2A	0.85434(7)	0.01392(7)	0.08663(2)	0.0203(2)
O2A	0.86211(5)	-0.03730(5)	0.07388(2)	0.02269(17)
N3A	0.77788(6)	-0.00986(6)	0.09705(2)	0.0233(2)
C4A	0.93030(7)	0.16545(8)	0.10079(2)	0.0283(2)
O4A	0.99693(6)	0.23934(6)	0.10105(2)	0.0430(3)
C5A	0.84693(8)	0.14459(8)	0.11322(2)	0.0288(3)
C6A	0.77032(7)	0.04945(7)	0.10963(2)	0.0257(2)
O6A	0.69925(6)	0.02641(6)	0.11906(2)	0.0357(2)
C7A	0.87086(10)	0.15550(10)	0.13737(2)	0.0440(3)
H7A1	0.916811	0.218260	0.140065	0.053*
H7A2	0.817247	0.143112	0.145696	0.053*
C8A	0.90497(13)	0.09579(13)	0.14560(2)	0.0573(4)
H8A1	0.918460	0.106849	0.160930	0.086*
H8A2	0.859373	0.033311	0.143422	0.086*
H8A3	0.959125	0.108600	0.137780	0.086*
C9A	0.81724(9)	0.21156(8)	0.10660(2)	0.0381(3)
H9A1	0.764212	0.199575	0.115128	0.046*
H9A2	0.865416	0.272502	0.110139	0.046*
C10A	0.79484(10)	0.20792(10)	0.08288(2)	0.0438(3)
H10A	0.776594	0.251920	0.079797	0.066*
H10B	0.847417	0.221250	0.074295	0.066*
H10C	0.746104	0.148245	0.079290	0.066*
C1B	0.81613(8)	0.16813(8)	0.02760(2)	0.0280(2)
O1B	0.73048(6)	0.15167(7)	0.02760(2)	0.0412(2)
H1B	0.6988(12)	0.1009(12)	0.0338(3)	0.049*

C2B	0.84057(8)	0.11056(8)	0.03695(2)	0.0277(2)
H2B	0.797354	0.058400	0.044133	0.033*
C3B	0.92836(7)	0.12966(7)	0.03572(2)	0.0242(2)
H3B	0.944481	0.090097	0.042174	0.029*
C4B	0.99335(7)	0.20534(7)	0.02526(2)	0.0225(2)
C5B	0.96781(8)	0.26311(7)	0.01629(2)	0.0251(2)
H5B	1.011077	0.315500	0.009193	0.030*
C6B	0.88050(8)	0.24543(7)	0.01756(2)	0.0271(2)
H6B	0.864705	0.286034	0.011573	0.033*
C7B	1.08700(7)	0.22177(8)	0.02286(2)	0.0252(2)
H7B1	1.100094	0.222351	0.007395	0.030*
H7B2	1.089978	0.171388	0.029464	0.030*
C8B	1.15893(7)	0.30804(7)	0.03286(2)	0.0247(2)
H8B1	1.218204	0.316345	0.029228	0.030*
H8B2	1.155145	0.358772	0.026767	0.030*
N2B	1.14965(6)	0.30775(6)	0.05673(2)	0.0215(2)
H21	1.2027(7)	0.3499(8)	0.0626(2)	0.032*
H22	1.1346(9)	0.2538(7)	0.0624(2)	0.032*
H23	1.1085(8)	0.3224(10)	0.0606(2)	0.032*

Table S11 Atomic displacement parameters of (II) (Å^2).

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1A	0.0191(4)	0.0245(5)	0.0243(4)	0.0005(3)	0.0037(3)	0.0074(4)
C2A	0.0219(5)	0.0216(5)	0.0179(5)	0.0026(4)	-0.0012(4)	0.0112(4)
O2A	0.0260(4)	0.0244(4)	0.0199(4)	-0.0006(3)	-0.0004(3)	0.0144(3)
N3A	0.0216(4)	0.0205(4)	0.0245(4)	0.0006(3)	0.0029(3)	0.0081(4)
C4A	0.0238(5)	0.0244(5)	0.0300(6)	-0.0019(4)	0.0006(4)	0.0070(4)
O4A	0.0272(5)	0.0272(4)	0.0592(6)	-0.0096(4)	0.0052(4)	0.0020(4)
C5A	0.0281(6)	0.0238(5)	0.0291(6)	-0.0049(4)	0.0050(4)	0.0090(5)

C6A	0.0253(5)	0.0233(5)	0.0264(5)	0.0016(4)	0.0048(4)	0.0106(4)
O6A	0.0291(4)	0.0296(4)	0.0444(5)	0.0010(4)	0.0158(4)	0.0117(4)
C7A	0.0461(8)	0.0439(8)	0.0301(6)	-0.0116(5)	0.0017(6)	0.0137(6)
C8A	0.0635(10)	0.0723(11)	0.0296(7)	-0.0014(7)	-0.0061(7)	0.0290(9)
C9A	0.0379(7)	0.0240(6)	0.0505(8)	-0.0009(5)	0.0142(6)	0.0141(5)
C10A	0.0432(8)	0.0359(7)	0.0564(8)	0.0077(6)	0.0059(6)	0.0229(6)
C1B	0.0252(5)	0.0311(6)	0.0284(5)	0.0041(4)	0.0006(4)	0.0144(5)
O1B	0.0269(4)	0.0414(5)	0.0565(6)	0.0211(4)	0.0078(4)	0.0180(4)
C2B	0.0275(5)	0.0276(5)	0.0251(5)	0.0070(4)	0.0026(4)	0.0116(5)
C3B	0.0288(5)	0.0271(5)	0.0176(5)	0.0011(4)	-0.0020(4)	0.0147(4)
C4B	0.0249(5)	0.0251(5)	0.0146(4)	-0.0046(4)	-0.0023(4)	0.0103(4)
C5B	0.0281(5)	0.0213(5)	0.0202(5)	-0.0006(4)	0.0005(4)	0.0082(4)
C6B	0.0319(6)	0.0252(5)	0.0251(5)	0.0025(4)	-0.0011(4)	0.0149(5)
C7B	0.0255(5)	0.0291(5)	0.0184(5)	-0.0046(4)	-0.0001(4)	0.0116(4)
C8B	0.0233(5)	0.0277(5)	0.0174(5)	0.0000(4)	0.0005(4)	0.0085(4)
N2B	0.0222(4)	0.0222(4)	0.0185(4)	-0.0025(3)	-0.0015(3)	0.0100(4)

Table S12 Bond lengths in (II) (Å).

N1A—C4A	1.3610(15)	C10A—H10C	0.9800
N1A—C2A	1.3905(13)	C1B—O1B	1.3649(14)
N1A—H1A	0.880(9)	C1B—C2B	1.3923(16)
C2A—O2A	1.2484(13)	C1B—C6B	1.3923(16)
C2A—N3A	1.3428(13)	O1B—H1B	0.862(19)
N3A—C6A	1.3508(14)	C2B—C3B	1.3885(16)
C4A—O4A	1.2230(14)	C2B—H2B	0.9500
C4A—C5A	1.5159(16)	C3B—C4B	1.3921(15)
C5A—C6A	1.5310(15)	C3B—H3B	0.9500
C5A—C9A	1.5432(18)	C4B—C5B	1.3983(16)
C5A—C7A	1.5486(18)	C4B—C7B	1.5090(15)

C6A—O6A	1.2373(14)	C5B—C6B	1.3884(16)
C7A—C8A	1.516(3)	C5B—H5B	0.9500
C7A—H7A1	0.9900	C6B—H6B	0.9500
C7A—H7A2	0.9900	C7B—C8B	1.5219(15)
C8A—H8A1	0.9800	C7B—H7B1	0.9900
C8A—H8A2	0.9800	C7B—H7B2	0.9900
C8A—H8A3	0.9800	C8B—N2B	1.4972(13)
C9A—C10A	1.523(2)	C8B—H8B1	0.9900
C9A—H9A1	0.9900	C8B—H8B2	0.9900
C9A—H9A2	0.9900	N2B—H21	0.918(9)
C10A—H10A	0.9800	N2B—H22	0.909(9)
C10A—H10B	0.9800	N2B—H23	0.902(9)

Table S13 Valence angles in (II) (°).

C4A—N1A—C2A	124.99(9)	C9A—C10A—H10C	109.5
C4A—N1A—H1A	117.6(9)	H10A—C10A—H10C	109.5
C2A—N1A—H1A	117.4(9)	H10B—C10A—H10C	109.5
O2A—C2A—N3A	122.07(9)	O1B—C1B—C2B	109.5
O2A—C2A—N1A	116.66(9)	O1B—C1B—C6B	122.66(11)
N3A—C2A—N1A	121.26(9)	C2B—C1B—C6B	117.76(10)
C2A—N3A—C6A	120.27(9)	C1B—O1B—H1B	119.58(10)
O4A—C4A—N1A	120.73(11)	C3B—C2B—C1B	106.5(12)
O4A—C4A—C5A	122.11(11)	C3B—C2B—H2B	119.74(10)
N1A—C4A—C5A	117.15(9)	C1B—C2B—H2B	120.1
C4A—C5A—C6A	113.11(9)	C2B—C3B—C4B	120.1
C4A—C5A—C9A	108.71(10)	C2B—C3B—H3B	121.66(10)
C6A—C5A—C9A	109.60(10)	C4B—C3B—H3B	119.2
C4A—C5A—C7A	107.63(10)	C3B—C4B—C5B	119.2
C6A—C5A—C7A	107.99(10)	C3B—C4B—C7B	117.74(10)

C9A—C5A—C7A	109.75(10)	C5B—C4B—C7B	120.78(10)
O6A—C6A—N3A	119.35(10)	C6B—C5B—C4B	121.42(10)
O6A—C6A—C5A	117.77(10)	C6B—C5B—H5B	121.33(10)
N3A—C6A—C5A	122.87(9)	C4B—C5B—H5B	119.3
C8A—C7A—C5A	114.73(11)	C5B—C6B—C1B	119.3
C8A—C7A—H7A1	108.6	C5B—C6B—H6B	119.91(10)
C5A—C7A—H7A1	108.6	C1B—C6B—H6B	120.0
C8A—C7A—H7A2	108.6	C4B—C7B—C8B	120.0
C5A—C7A—H7A2	108.6	C4B—C7B—H7B1	114.87(9)
H7A1—C7A—H7A2	107.6	C8B—C7B—H7B1	108.6
C7A—C8A—H8A1	109.5	C4B—C7B—H7B2	108.6
C7A—C8A—H8A2	109.5	C8B—C7B—H7B2	108.6
H8A1—C8A—H8A2	109.5	H7B1—C7B—H7B2	108.6
C7A—C8A—H8A3	109.5	N2B—C8B—C7B	107.5
H8A1—C8A—H8A3	109.5	N2B—C8B—H8B1	111.73(8)
H8A2—C8A—H8A3	109.5	C7B—C8B—H8B1	109.3
C10A—C9A—C5A	113.74(10)	N2B—C8B—H8B2	109.3
C10A—C9A—H9A1	108.8	C7B—C8B—H8B2	109.3
C5A—C9A—H9A1	108.8	H8B1—C8B—H8B2	109.3
C10A—C9A—H9A2	108.8	C8B—N2B—H21	107.9
C5A—C9A—H9A2	108.8	C8B—N2B—H22	109.5(9)
H9A1—C9A—H9A2	107.7	H21—N2B—H22	111.5(9)
C9A—C10A—H10A	109.5	C8B—N2B—H23	108.7(13)
C9A—C10A—H10B	109.5	H21—N2B—H23	111.4(9)
H10A—C10A—H10B	124.99(9)	H22—N2B—H23	106.7(13)

Table S14 Torsion angles in (II) (°).

C4A—N1A—C2A—O2A	172.61(10)	C4A—C5A—C7A—C8A	-59.32(15)
C4A—N1A—C2A—N3A	-6.86(16)	C6A—C5A—C7A—C8A	63.10(15)

O2A—C2A—N3A—C6A	-175.65(10)	C9A—C5A—C7A—C8A	-177.47(12)
N1A—C2A—N3A—C6A	3.79(15)	C4A—C5A—C9A—C10A	60.80(14)
C2A—N1A—C4A—O4A	-174.19(11)	C6A—C5A—C9A—C10A	-63.29(13)
C2A—N1A—C4A—C5A	6.79(16)	C7A—C5A—C9A—C10A	178.27(11)
O4A—C4A—C5A—C6A	177.05(12)	O1B—C1B—C2B—C3B	177.69(11)
N1A—C4A—C5A—C6A	-3.95(15)	C6B—C1B—C2B—C3B	-1.52(17)
O4A—C4A—C5A—C9A	55.07(16)	C1B—C2B—C3B—C4B	-0.18(17)
N1A—C4A—C5A—C9A	-125.93(11)	C2B—C3B—C4B—C5B	1.23(15)
O4A—C4A—C5A—C7A	-63.75(15)	C2B—C3B—C4B—C7B	-175.99(10)
N1A—C4A—C5A—C7A	115.26(12)	C3B—C4B—C5B—C6B	-0.60(15)
C2A—N3A—C6A—O6A	179.77(10)	C7B—C4B—C5B—C6B	176.60(10)
C2A—N3A—C6A—C5A	-1.47(16)	C4B—C5B—C6B—C1B	-1.08(17)
C4A—C5A—C6A—O6A	-179.67(10)	O1B—C1B—C6B—C5B	-177.11(11)
C9A—C5A—C6A—O6A	-58.19(14)	C2B—C1B—C6B—C5B	2.14(17)
C7A—C5A—C6A—O6A	61.33(14)	C3B—C4B—C7B—C8B	-120.76(11)
C4A—C5A—C6A—N3A	1.55(16)	C5B—C4B—C7B—C8B	62.13(13)
C9A—C5A—C6A—N3A	123.03(12)	C4B—C7B—C8B—N2B	64.82(12)
C7A—C5A—C6A—N3A	-117.45(12)	C4A—C5A—C7A—C8A	-59.32(15)