

**A new supramolecular semi conductor cobalt organometallic complex:
structural study, optical and electrical properties**

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Table. S1. Fractional atomic coordinates and equivalent thermal factors (U_{eq}) or isotropic (U_{iso}) for $[\text{Co}(\text{C}_3\text{H}_7\text{NO})_6][\text{CoBr}_{1.93}\text{Cl}_{2.07}]$.

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Co1	1.0000	1.0000	0.5000	0.01788 (13)	
O1	0.92336 (12)	0.89330 (16)	0.55466 (9)	0.0243 (4)	
C2	0.90235 (17)	0.9004 (3)	0.61441 (14)	0.0243 (6)	
N3	0.91880 (15)	0.9964 (2)	0.65461 (11)	0.0302 (6)	
H3A	0.9456	1.0590	0.6396	0.036*	
H3B	0.9029	0.9979	0.6965	0.036*	
C4	0.8572 (2)	0.7946 (3)	0.64150 (16)	0.0432 (9)	
H4A	0.8016	0.7787	0.6100	0.052*	
H4B	0.8429	0.8139	0.6885	0.052*	
C5	0.9136 (3)	0.6833 (3)	0.64603 (18)	0.0615 (12)	
H5A	0.9299	0.6660	0.5999	0.092*	
H5B	0.8810	0.6148	0.6611	0.092*	
H5C	0.9666	0.6967	0.6800	0.092*	
O6	0.89592 (12)	1.04311 (16)	0.42358 (9)	0.0238 (4)	
C7	0.83417 (18)	0.9800 (3)	0.39279 (14)	0.0257 (7)	
N8	0.81336 (15)	0.8741 (2)	0.41616 (12)	0.0348 (6)	
H8A	0.8431	0.8447	0.4549	0.042*	
H8B	0.7697	0.8328	0.3931	0.042*	
C9	0.7815 (2)	1.0273 (3)	0.32700 (15)	0.0386 (8)	
H9A	0.7545	1.1052	0.3369	0.046*	
H9B	0.7339	0.9699	0.3102	0.046*	
C10	0.8382 (3)	1.0450 (4)	0.27104 (17)	0.0715 (13)	
H10A	0.8857	1.1011	0.2879	0.107*	
H10B	0.8028	1.0781	0.2289	0.107*	
H10C	0.8629	0.9673	0.2598	0.107*	
O11	0.97988 (11)	1.15812 (16)	0.55731 (9)	0.0221 (4)	
C12	0.95248 (16)	1.2620 (3)	0.54012 (14)	0.0223 (6)	
N13	0.91294 (15)	1.2881 (2)	0.47648 (11)	0.0302 (6)	
H13A	0.9049	1.2315	0.4442	0.036*	
H13B	0.8946	1.3620	0.4663	0.036*	
C14	0.96412 (19)	1.3634 (3)	0.59238 (14)	0.0306 (7)	
H14A	1.0035	1.4245	0.5765	0.037*	
H14B	0.9066	1.4023	0.5931	0.037*	
C15	1.0008 (2)	1.3260 (3)	0.66539 (15)	0.0477 (9)	
H15A	0.9595	1.2715	0.6835	0.072*	
H15B	1.0101	1.3976	0.6954	0.072*	

H15C	1.0567	1.2844	0.6651	0.072*
Co2	0.5000	0.0000	0.5000	0.01870 (13)
O21	0.39070 (11)	-0.10824 (16)	0.46535 (9)	0.0231 (4)
C22	0.33503 (18)	-0.1085 (2)	0.41155 (14)	0.0231 (6)
N23	0.32646 (15)	-0.0184 (2)	0.36591 (12)	0.0327 (6)
H23A	0.3610	0.0449	0.3731	0.039*
H23B	0.2863	-0.0220	0.3285	0.039*
C24	0.2715 (2)	-0.2110 (3)	0.39701 (16)	0.0393 (8)
H24A	0.2586	-0.2235	0.3457	0.047*
H24B	0.2160	-0.1881	0.4133	0.047*
C25	0.3030 (2)	-0.3283 (3)	0.43114 (16)	0.0404 (8)
H25A	0.3600	-0.3491	0.4179	0.061*
H25B	0.2607	-0.3922	0.4156	0.061*
H25C	0.3089	-0.3199	0.4821	0.061*
O26	0.53241 (12)	-0.01159 (16)	0.39824 (9)	0.0222 (4)
C27	0.55555 (17)	0.0726 (3)	0.36109 (13)	0.0216 (6)
N28	0.59604 (14)	0.1692 (2)	0.38937 (11)	0.0285 (6)
H28A	0.6076	0.1762	0.4352	0.034*
H28B	0.6116	0.2268	0.3624	0.034*
C29	0.53710 (19)	0.0612 (3)	0.28301 (14)	0.0330 (8)
H29A	0.4734	0.0488	0.2694	0.040*
H29B	0.5667	-0.0124	0.2695	0.040*
C30	0.5644 (2)	0.1661 (3)	0.24004 (14)	0.0421 (9)
H30A	0.5330	0.2392	0.2503	0.063*
H30B	0.5503	0.1471	0.1901	0.063*
H30C	0.6276	0.1795	0.2521	0.063*
O31	0.43295 (11)	0.15700 (16)	0.46531 (9)	0.0227 (4)
C32	0.42225 (17)	0.2534 (3)	0.49611 (14)	0.0236 (6)
N33	0.42960 (15)	0.2612 (2)	0.56534 (11)	0.0304 (6)
H33A	0.4425	0.1966	0.5914	0.036*
H33B	0.4216	0.3309	0.5852	0.036*
C34	0.4023 (2)	0.3692 (3)	0.45640 (14)	0.0415 (9)
H34A	0.3543	0.4109	0.4753	0.050*
H34B	0.4546	0.4218	0.4650	0.050*
C35	0.37639 (19)	0.3548 (3)	0.37877 (14)	0.0343 (7)
H35A	0.4245	0.3171	0.3589	0.051*
H35B	0.3636	0.4342	0.3573	0.051*
H35C	0.3242	0.3037	0.3694	0.051*
Co3	0.73726 (2)	0.53204 (3)	0.35486 (2)	0.02224 (11)

Br1	0.81580 (2)	0.39062 (3)	0.29299 (2)	0.03443 (14)	0.766 (2)
Cl1	0.81580 (2)	0.39062 (3)	0.29299 (2)	0.03443 (14)	0.234 (2)
Br2	0.82027 (3)	0.57717 (4)	0.46508 (2)	0.02985 (17)	0.487 (2)
Cl2	0.82027 (3)	0.57717 (4)	0.46508 (2)	0.02985 (17)	0.513 (2)
Br3	0.70011 (3)	0.70585 (4)	0.28451 (2)	0.03086 (16)	0.568 (2)
Cl3	0.70011 (3)	0.70585 (4)	0.28451 (2)	0.03086 (16)	0.432 (2)
Br4	0.60502 (4)	0.45625 (5)	0.37400 (3)	0.0287 (2)	0.112 (2)
Cl4	0.60502 (4)	0.45625 (5)	0.37400 (3)	0.0287 (2)	0.888 (2)

Table. S2. Anisotropic thermal stirring factors.

	<i>U</i> ¹¹	<i>U</i> ²²	<i>U</i> ³³	<i>U</i> ¹²	<i>U</i> ¹³	<i>U</i> ²³
Co1	0.0214 (3)	0.0159 (3)	0.0167 (3)	-0.0007 (2)	0.0039 (2)	0.0004 (2)
O1	0.0293 (11)	0.0253 (11)	0.0198 (10)	-0.0053 (9)	0.0083 (9)	0.0012 (8)
C2	0.0177 (15)	0.0282 (17)	0.0265 (16)	0.0034 (13)	0.0020 (13)	0.0054 (13)
N3	0.0378 (15)	0.0320 (15)	0.0228 (13)	-0.0023 (12)	0.0111 (12)	0.0018 (11)
C4	0.050 (2)	0.046 (2)	0.0372 (19)	-0.0204 (18)	0.0197 (17)	0.0044 (16)
C5	0.117 (4)	0.029 (2)	0.043 (2)	-0.008 (2)	0.026 (2)	0.0079 (17)
O6	0.0262 (11)	0.0182 (11)	0.0246 (10)	-0.0008 (9)	-0.0039 (9)	0.0003 (8)
C7	0.0239 (16)	0.0264 (17)	0.0267 (16)	0.0054 (14)	0.0038 (13)	0.0008 (13)
N8	0.0314 (14)	0.0325 (16)	0.0363 (15)	-0.0083 (12)	-0.0087 (12)	0.0040 (12)
C9	0.0352 (18)	0.0303 (19)	0.044 (2)	-0.0015 (15)	-0.0153 (16)	0.0044 (15)
C10	0.086 (3)	0.102 (4)	0.0260 (19)	0.044 (3)	0.007 (2)	0.009 (2)
O11	0.0279 (11)	0.0160 (10)	0.0229 (10)	0.0024 (9)	0.0051 (8)	-0.0012 (8)
C12	0.0164 (14)	0.0240 (17)	0.0284 (16)	-0.0015 (12)	0.0091 (13)	-0.0020 (13)
N13	0.0431 (15)	0.0199 (14)	0.0254 (13)	0.0086 (12)	-0.0016 (12)	-0.0013 (11)
C14	0.0324 (17)	0.0230 (17)	0.0366 (18)	0.0007 (14)	0.0055 (15)	-0.0099 (14)
C15	0.067 (3)	0.041 (2)	0.0328 (19)	0.0010 (18)	-0.0005 (18)	-0.0161 (16)
Co2	0.0231 (3)	0.0157 (3)	0.0168 (3)	0.0004 (2)	0.0014 (2)	-0.0016 (2)
O21	0.0254 (10)	0.0218 (11)	0.0201 (10)	-0.0038 (8)	-0.0033 (9)	-0.0003 (8)
C22	0.0236 (15)	0.0223 (16)	0.0240 (15)	0.0044 (13)	0.0056 (13)	-0.0014 (12)
N23	0.0279 (14)	0.0344 (16)	0.0321 (14)	-0.0070 (12)	-0.0072 (12)	0.0103 (12)
C24	0.0383 (19)	0.0320 (19)	0.0422 (19)	-0.0118 (15)	-0.0109 (16)	0.0039 (15)
C25	0.042 (2)	0.0282 (19)	0.049 (2)	-0.0098 (15)	-0.0006 (17)	0.0015 (16)
O26	0.0291 (11)	0.0173 (11)	0.0206 (10)	0.0017 (9)	0.0048 (9)	0.0000 (8)
C27	0.0197 (15)	0.0237 (16)	0.0216 (15)	0.0053 (13)	0.0037 (13)	-0.0020 (13)
N28	0.0389 (15)	0.0267 (15)	0.0205 (12)	-0.0054 (12)	0.0067 (11)	0.0030 (11)
C29	0.0259 (16)	0.051 (2)	0.0223 (15)	-0.0014 (15)	0.0026 (14)	0.0010 (14)

C30	0.0407 (19)	0.063 (2)	0.0219 (16)	0.0003 (18)	0.0018 (15)	0.0098 (16)
O31	0.0297 (11)	0.0163 (10)	0.0215 (10)	0.0032 (8)	0.0022 (9)	-0.0032 (8)
C32	0.0212 (15)	0.0234 (16)	0.0261 (15)	0.0003 (13)	0.0028 (13)	-0.0026 (13)
N33	0.0470 (16)	0.0200 (14)	0.0235 (13)	0.0099 (12)	0.0031 (12)	-0.0030 (11)
C34	0.072 (2)	0.0234 (18)	0.0302 (17)	0.0132 (17)	0.0106 (17)	0.0030 (14)
C35	0.0349 (18)	0.0310 (18)	0.0353 (18)	-0.0032 (15)	0.0001 (15)	0.0081 (14)
Co3	0.0240 (2)	0.0223 (2)	0.0197 (2)	-0.00151 (17)	0.00115 (17)	-0.00008 (16)
Br1	0.0394 (2)	0.0395 (3)	0.0253 (2)	0.00809 (18)	0.00778 (16)	-0.00436 (16)
Cl1	0.0394 (2)	0.0395 (3)	0.0253 (2)	0.00809 (18)	0.00778 (16)	-0.00436 (16)
Br2	0.0343 (3)	0.0248 (3)	0.0271 (3)	-0.00099 (19)	-0.00610 (19)	0.00283 (18)
Cl2	0.0343 (3)	0.0248 (3)	0.0271 (3)	-0.00099 (19)	-0.00610 (19)	0.00283 (18)
Br3	0.0379 (3)	0.0290 (3)	0.0237 (2)	-0.00602 (19)	-0.00134 (18)	0.00521 (17)
Cl3	0.0379 (3)	0.0290 (3)	0.0237 (2)	-0.00602 (19)	-0.00134 (18)	0.00521 (17)
Br4	0.0274 (4)	0.0226 (4)	0.0368 (4)	-0.0050 (3)	0.0073 (3)	-0.0003 (3)
Cl4	0.0274 (4)	0.0226 (4)	0.0368 (4)	-0.0050 (3)	0.0073 (3)	-0.0003 (3)

Table. S3. Attribution of the different modes of vibration relative to [Co(PM)₆][CoBr_{1.93}Cl_{2.07}] complex.

(IR) cm ⁻¹	Attribution
3421	$\nu_{as}(NH_2)$
3111	$\nu_s(NH_2)$
2962	$\nu_{as}(CH_3)$
2858	$\nu_s(CH_3)$
2807	$\nu_s(CH_2)$
2769	$\nu_s(CH_2)$
1658	$\nu C=O$
1570	$\beta(NH_2)$
1459	$\beta_{as}(CH_3) + \delta_{as}(CH_3)$
1410	$\beta(CH_2) + \beta_s(CH_3) + \nu(C-N)$
1376	$\beta_s(CH_3) + \delta_s(CH_3) + \omega(CH_2)$
1084	$\rho(CH_3) + \rho(CH_2) + t(CH_2)$
1006	$\nu_s(C-C) + \rho(CH_3) + \omega(CH_2)$
874	$\rho(CH_3) + t(CH_2) + \nu_s(C-C) + \pi_{Co}$

s: symmetric, as: asymmetric, v:stretching, β : bending, δ : scissoring, ρ : rocking, ω : wagging, t: twisting, π : out-of-plane bend.

Table. S4. Selected bond distances (\AA) and angles ($^\circ$) of $[\text{Co}(\text{PM})_6][\text{CoBr}_{1.93}\text{Cl}_{2.07}]$.

$[\text{Co1}(\text{C}_3\text{H}_7\text{NO})_6]^+$	
Co1—O1	2.0728 (17)
Co1—O1 ⁱ	2.0728 (17)
Co1—O6 ⁱ	2.0679 (17)
Co1—O6	2.0679 (17)
Co1—O11	2.1213 (17)
Co1—O11 ⁱ	2.1214 (17)
O1—C2	1.248 (3)
O6—C7	1.258 (3)
O11—C12	1.255 (3)
C2—N3	1.320 (3)
C7—N8	1.314 (3)
C12—N13	1.320 (3)
C2—C4	1.499 (4)
C4—C5	1.506 (4)
C7—C9	1.497 (4)
C9—C10	1.503 (4)
C12—C14	1.503 (4)
C14—C15	1.497 (4)
O6 ⁱ —Co1—O6	180.0
O6 ⁱ —Co1—O1	86.96 (7)
O6—Co1—O1	93.04 (7)
O6 ⁱ —Co1—O1 ⁱ	93.04 (7)
O6—Co1—O1 ⁱ	86.96 (7)
O1—Co1—O1 ⁱ	180.0
O6 ⁱ —Co1—O11	88.73 (7)
O6—Co1—O11	91.27 (7)
O1—Co1—O11	93.75 (7)
O1 ⁱ —Co1—O11	86.25 (7)
O6 ⁱ —Co1—O11 ⁱ	91.26 (7)
O6—Co1—O11 ⁱ	88.74 (7)
O1—Co1—O11 ⁱ	86.25 (7)
O1 ⁱ —Co1—O11 ⁱ	93.75 (7)
O11—Co1—O11 ⁱ	180.0
C2—O1—Co1	133.18 (18)
C7—O6—Co1	131.39 (18)
C12—O11—Co1	133.70 (17)
O1—C2—N3	122.7 (3)
O6—C7—N8	122.8 (3)
O11—C12—N13	122.5 (2)
O1—C2—C4	118.3 (3)

O1—C2—C4	118.3 (3)
O11—C12—C14	120.5 (2)
N3—C2—C4	119.0 (3)
N8—C7—C9	118.4 (3)
N13—C12—C14	117.0 (2)
C2—C4—C5	111.4 (3)
C7—C9—C10	110.8 (3)
C15—C14—C12	114.5 (2)
Co1—O1—C2—N3	9.6 (4)
Co1—O6—C7—N8	16.2 (4)
Co1—O11—C12—N13	13.3 (4)
Co1—O1—C2—C4	-169.95 (19)
Co1—O6—C7—C9	-164.29 (19)
Co1—O11—C12—C14	-166.48 (18)
O1—C2—C4—C5	60.8 (4)
O6—C7—C9—C10	61.8 (4)
O11—C12—C14—C15	-6.3 (4)
N3—C2—C4—C5	-118.8 (3)
N3—C2—C4—C5	-118.8 (3)
N13—C12—C14—C15	173.9 (3)

[Co2(C₃H₇NO)₆]⁺

Co2—O21 ⁱⁱ	2.0974 (17)
Co2—O21	2.0974 (17)
Co2—O26	2.1049 (17)
Co2—O26 ⁱⁱ	2.1049 (17)
Co2—O31	2.0838 (17)
Co2—O31 ⁱⁱ	2.0838 (17)
O21—C22	1.245 (3)
O26—C27	1.262 (3)
O31—C32	1.247 (3)
C22—N23	1.326 (3)
C27—N28	1.317 (3)
C32—N33	1.328 (3)
C22—C24	1.500 (4)
C24—C25	1.505 (4)
C27—C29	1.498 (4)
C29—C30	1.525 (4)
C32—C34	1.503 (4)
C34—C35	1.501 (4)
O31—Co2—O21	92.18 (7)
O31 ⁱⁱ —Co2—O21	87.82 (7)
O21 ⁱⁱ —Co2—O21	180.00 (6)
O31—Co2—O26	85.85 (7)
O31 ⁱⁱ —Co2—O26	94.15 (7)
O21 ⁱⁱ —Co2—O26	92.24 (7)
O21—Co2—O26	87.76 (7)
O31—Co2—O26 ⁱⁱ	94.15 (7)
O31 ⁱⁱ —Co2—O26 ⁱⁱ	85.85 (7)
O21 ⁱⁱ —Co2—O26 ⁱⁱ	87.76 (7)

O21—Co2—O26 ⁱⁱ	92.24 (7)
O26—Co2—O26 ⁱⁱ	180.0
C22—O21—Co2	133.56 (18)
C27—O26—Co2	127.90 (17)
C32—O31—Co2	131.17 (17)
O21—C22—N23	122.7 (3)
O26—C27—N28	121.6 (2)
O31—C32—N33	122.6 (3)
O21—C22—C24	120.5 (3)
O26—C27—C29	118.9 (2)
O31—C32—C34	121.4 (2)
N23—C22—C24	116.7 (3)
N28—C27—C29	119.5 (3)
N33—C32—C34	116.0 (2)
C22—C24—C25	114.4 (3)
C27—C29—C30	117.3 (3)
C35—C34—C32	115.0 (3)
Co2—O21—C22—N23	-11.8 (4)
Co2—O26—C27—N28	28.0 (4)
Co2—O31—C32—N33	-22.2 (4)
Co2—O21—C22—C24	170.54 (19)
Co2—O26—C27—C29	-152.55 (19)
Co2—O31—C32—C34	156.3 (2)
O21—C22—C24—C25	-25.1 (4)
O26—C27—C29—C30	178.8 (2)
O31—C32—C34—C35	13.3 (4)
N23—C22—C24—C25	157.2 (3)
N28—C27—C29—C30	-1.8 (4)
N33—C32—C34—C35	-168.2 (3)
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[Co₃Br_{1.93}Cl_{2.07}]²⁻	
Co3—Br1/Cl1	2.4084 (5)
Co3—Br2/Cl2	2.3672 (6)
Co3—Br3/Cl3	2.3779 (5)
Co3—Br4/Br4	2.2907 (7)
Br4/Cl4—Co3—Br2/Cl2	107.91 (2)
Br4/Cl4—Co3—Br3/Cl3	104.21 (2)
Br2/Cl2—Co3—Br3/Cl3	113.20 (2)
Br4/Cl4—Co3—Br1/Cl1	111.73 (2)
Br2/Cl2—Co3—Br1/Cl1	109.81 (2)
Br3/Cl3—Co3—Br1/Cl1	109.88 (2)

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $-x+1, -y, -z+1$.

Fig. S1. Scanning electron microscope analysis spectrum of $[\text{Co}(\text{PM})_6][\text{CoBr}_{1.93}\text{Cl}_{2.07}]$.

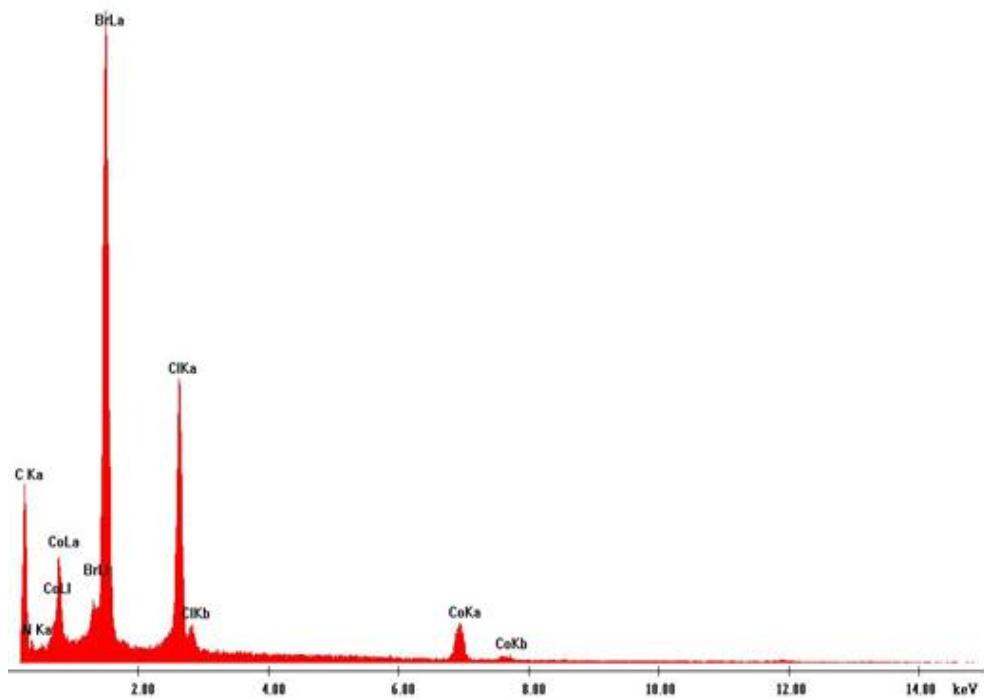


Fig. S2. IR absorption spectrum of the title complex.

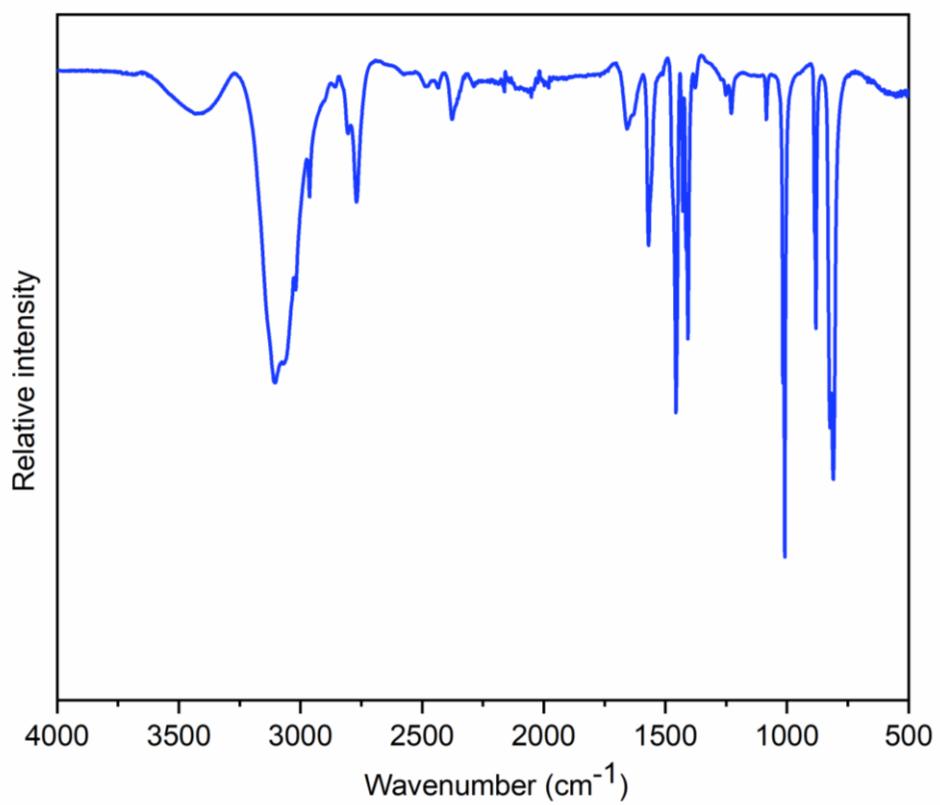


Fig. S3. The 3D representation of the Hirshfeld surface of (a) cationic part and (b) anionic, mapped with d_{norm} of $[\text{Co}(\text{PM})_6][\text{CoBr}_{1.93}\text{Cl}_{2.07}]$.

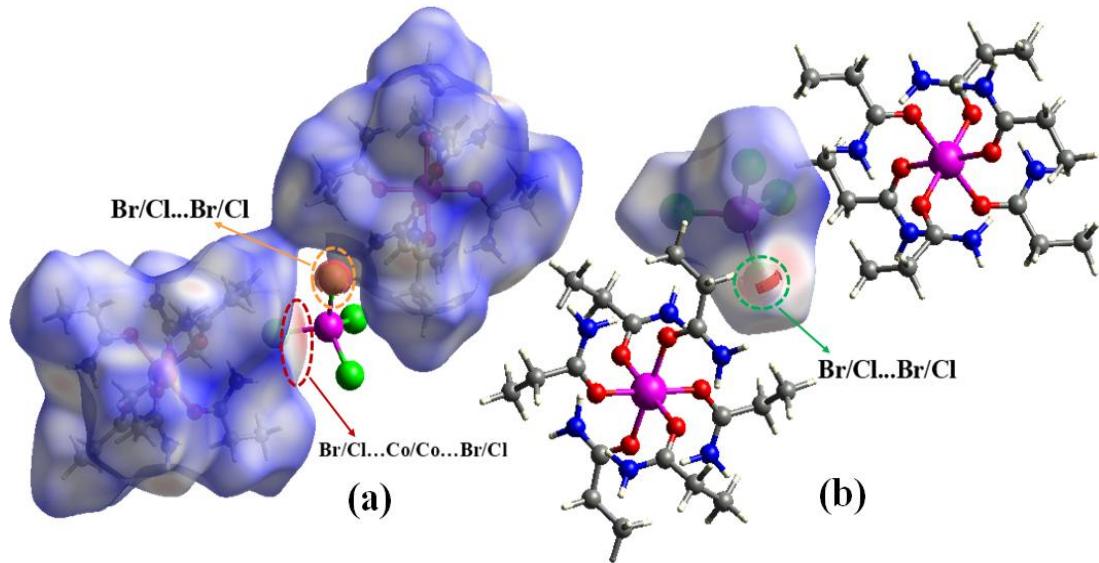


Fig. S4(a). The 2D-fingerprint plots with the relative contributions of the different intermolecular contacts percentages to the hirshfeld surface area occurring in $[\text{Co}_{1/2}(\text{PM})_6]^{2+}$ cationic part of $[\text{Co}(\text{PM})_6][\text{CoBr}_{1.93}\text{Cl}_{2.07}]$.

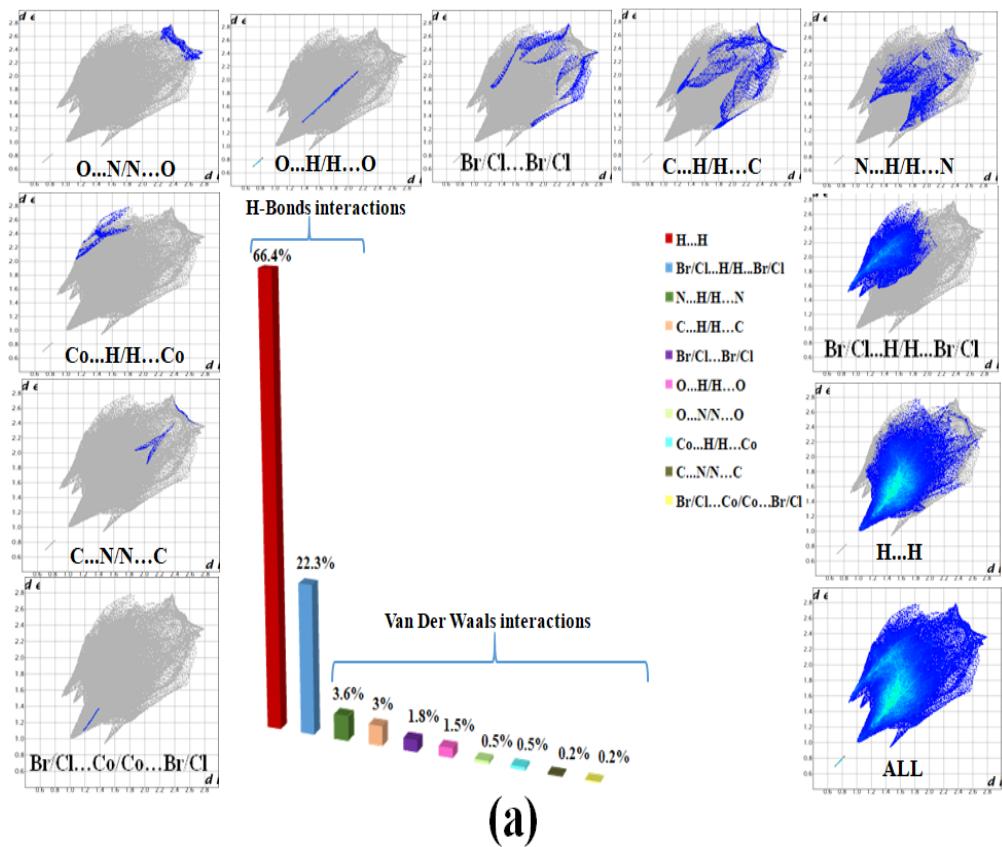
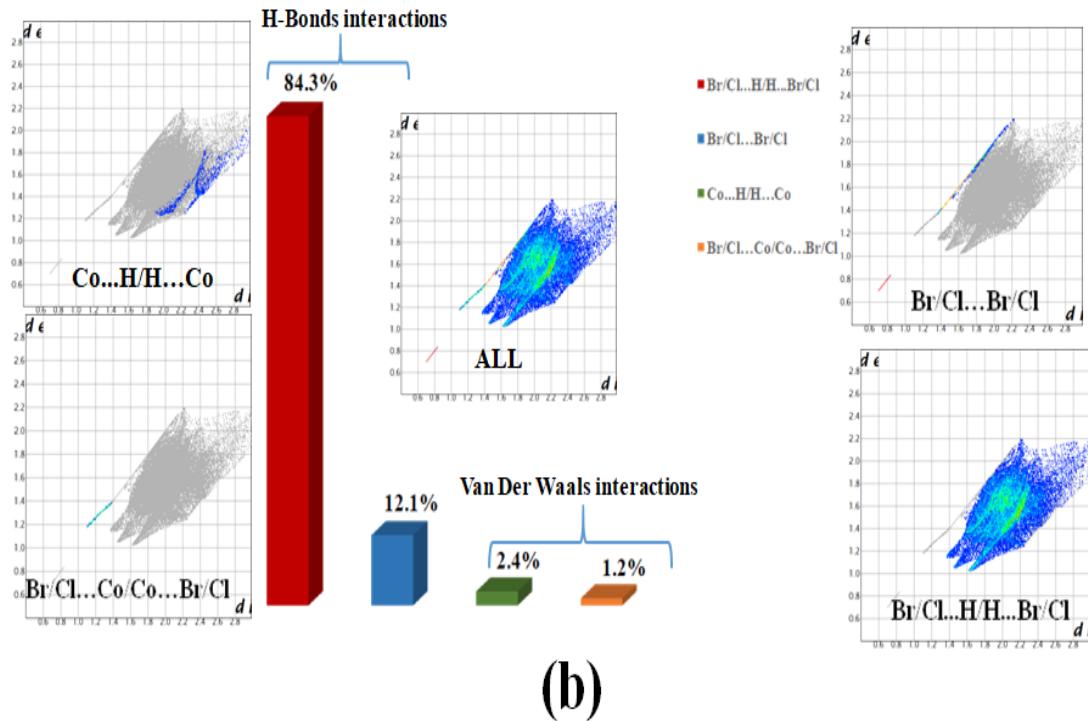


Fig. S4(b). The 2D-fingerprint plots with the relative contributions of the different intermolecular contacts percentages to the hirshfeld surface area occurring in $[\text{Co}(\text{BrCl})_4]^{2-}$ anionic part.



(b)

Fig. S5. Variation of the real part M' of the complex modulus as a function of the frequency at various temperatures.

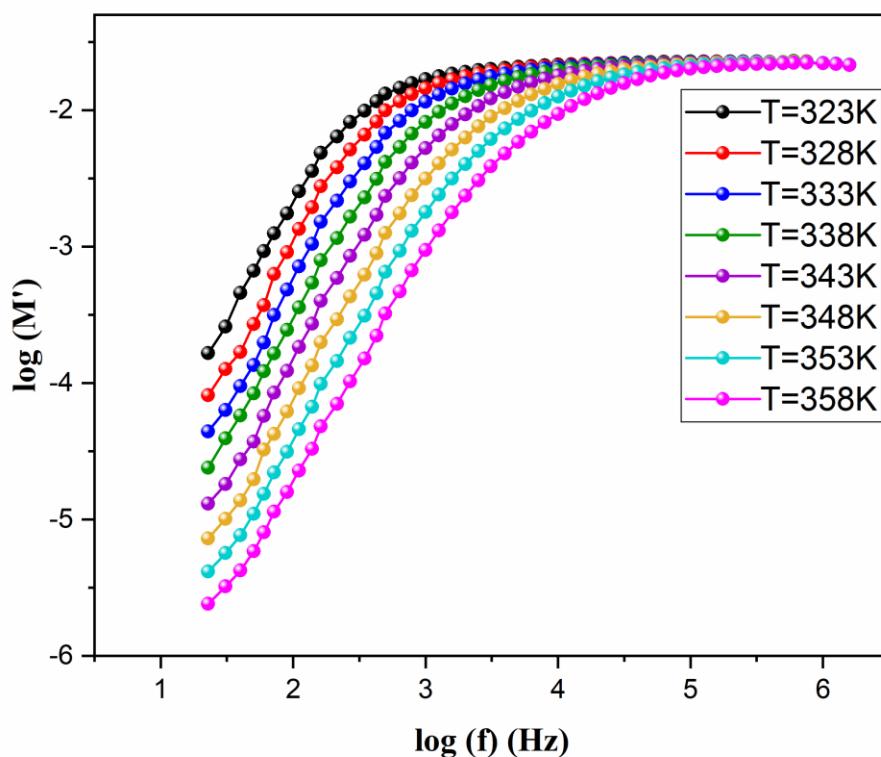


Fig. S6. 3D presentations of the imaginary part of (M''/M''_{\max}) versus frequency for different temperatures.

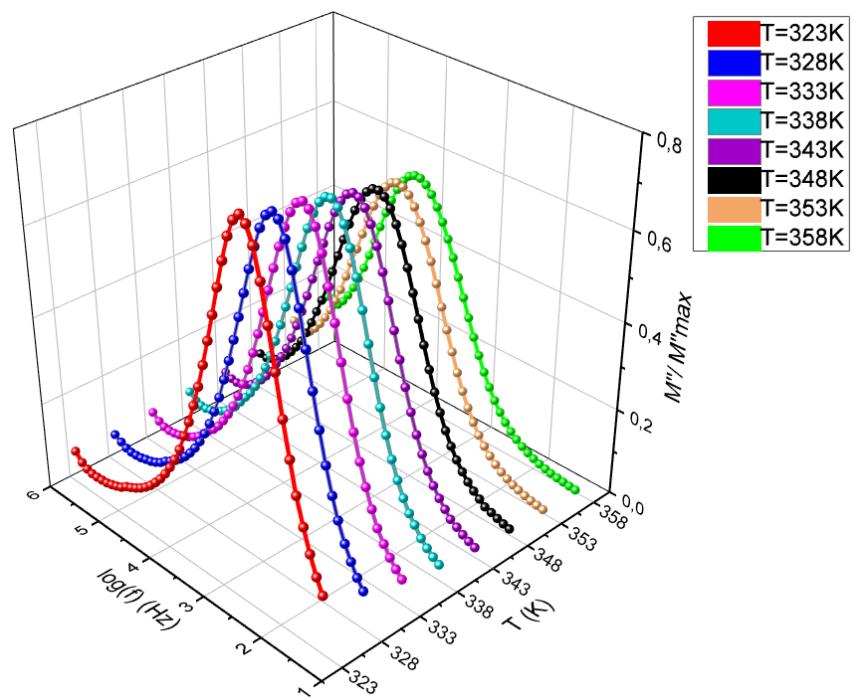


Fig. S7. Variation of ($\log (f_p)$) versus $1000/T$ of the $[\text{Co}(\text{PM})_6][\text{CoBr}_{1.93}\text{Cl}_{2.07}]$ complex.

