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Herz radicals: chemistry and materials science

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Table S1 Conductivity and magnetism of solids formed by Herz radicals.

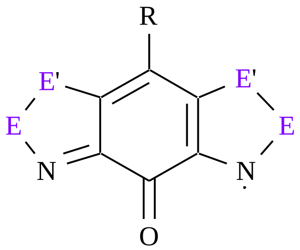
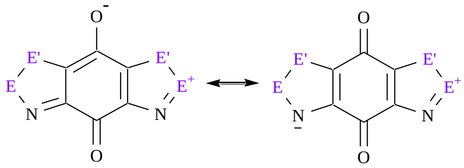
Radical	Conductivity[a]		Magnetism (T)[b,c]
	σ, S cm^{-1}	E_a eV	
1	2	3	4
	**E = E' = S**: 4×10^{-2}, 2×10^{-2} (R = NO_2, polymorphic MeCN solvates); 2×10^{-2} (R = NO_2, EtCN solvate; F); 6×10^{-3} (R = H); 10 (8 GPa) (R = NO_2, MeCN solvate) [S3,S5]; 3×10^{-3} (R = Cl; MeCN solvate); 4×10^{-3} (R = Cl); 3×10^{-5} (R = Ph) [S1,S2]; 6×10^{-5} (R = OAc); 6×10^{-4} (R = OMe); 9×10^{-4} (R = SMe) [S7]	**E = E' = S**: 0.05-0.09 (R = NO_2, polymorphic MeCN solvates); 0.10, ~0 (3 GPa) (R = F); 0.14 (R = NO_2, EtCN solvate); 0.16, ~0 (4 GPa) (R = H) [S3-S6]; 0.11 (R = Cl; MeCN solvate); 0.16 (R = Cl); 0.20 (R = Ph) [S1,S2]; 0.24 (R = OAc); 0.21 (R = OMe); 0.27 (R = SMe) [S7]	**E = E' = S**: T_N = 8.0^d (R = Cl), 4.5^d (R = Ph), 13 (R = F), 4^d (R = H) [S1-S4]
	**E = E' = S**: 10^{-3}; > 10 (8 GPa), 10^2 (12 GPa) [S8]	**E = E' = S**: 0.14, ~0 (8 GPa) [S8]	–

Table S1 *(continued)*

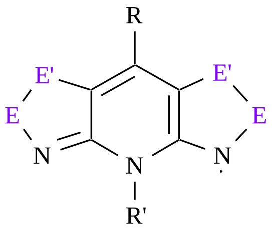
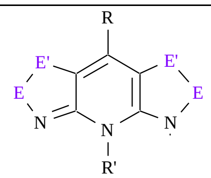
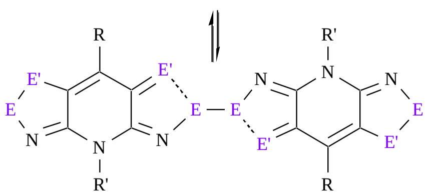
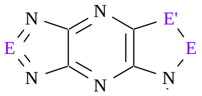
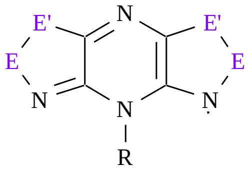
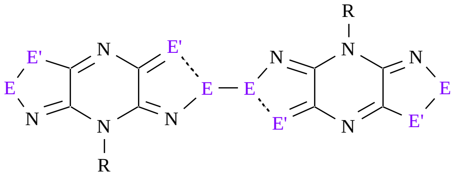
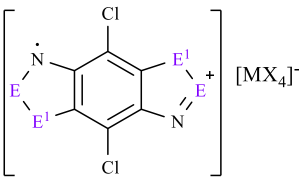
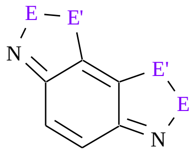
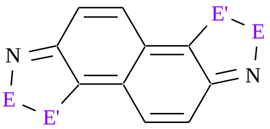
1	2	3	4
	**E = E' = S**: 5.3×10^{-6} (R = Cl, R' = Me) [S9]; 3.2×10^{-6} (R = Cl, R' = Et) [S10]; 4×10^{-7} (R = Cl, R' = Pr) [S10]; 2.3×10^{-6} (R = H, R' = Me) [S14,S15]; 10^{-5} (R = Me, R' = Me, Ph) [S16]; 7.5×10^{-6} (R = H, R' = Et) [S15]	**E = E' = S**: 0.40 (R = Cl, R' = Me) [S10]; 0.43 (R = Cl, R' = Et) [S10,S12]; 0.48 (R = Cl, R' = Pr) [S10]; 0.41 (R = Me, Et, R' = H) [S14,S15]	**E = E' = S**: T_N < 7[d] (R = Cl, R' = Me) [S9]; < 2 (R = Ph, R' = Me) [S11]; T_N / T_C ~5[e] (R = H, R' = Me) [S13]
	E = Se, E' = S: 2.1×10^{-3}, 0.5 (5 GPa) (R = Cl; R' = Me) [S9]; 10^{-4} (R = Cl, R' = Et) [S12,S17]; 5×10^{-6}; 10^{-3} (4-5 GPa) (R = Ph, R' = Et) [S21]; 7×10^{-6} (R = H, R' = Et) [S20]; 1.0×10^{-4}, 5.0×10^{-5}, 1.8×10^{-5} (R = Cl, R' = Et, Pr, CH_2CF_3, resp.); 1.9×10^{-4}, 1.2×10^{-4} (R = Me, Br, resp, R' = Et) [S18]; 2.3×10^{-6}, 10^{-1} (4 GPa), 10 (5 GPa) (R = H, R' = Me); 5.8×10^{-7}, 10^{-2} (4 GPa) (R = H, R' = Et) [S22,S23]; 10^{-6}, 1 (5 GPa) (R^1 = Me, R = F); 10^{-6}, 10^{-1} (5 GPa) (R = R' = Me) [S23]	**E = Se, E' = S**: 0.20 (R = Cl, R' = Me) [S9]; 0.27 (R = Cl, R' = Et) [S12,S17]; 0.32, 0.03 (5 GPa) (R = H, R' = Me); 0.36 (R = H, R' = Et) [S22]	**E = Se, E' = S**: T_C = 14.1, 13.6, 12.8 (R = Br, Me, Cl, resp., R' = Et) [S17-S19]; T_N = 18[f] (R = H, R' = Et) [S20]
	E = S, E' = Se 3×10^{-4} (R = H, R^1 = Me) [S24]; 3.5×10^{-5} (R = Cl, R' = Me) [S9]; 2.2×10^{-5} (R = Cl, R' = Et) [S12]	**E = S, E' = Se**: 0.24 (R = Me, R' = H) [S24]; 0.30 (R = Cl, R' = Me) [S9]; 0.31 (R = Cl, R' = Et) [S12]	**E = S, E' = Se**: T_N = 14[d] (R = Cl, R' = Et) [S19]
	E = E' = Se: 4.3×10^{-3}, 2 (5 GPa) (R = Cl, R' = Me) [S9]; 10^{-3} (R = Me, R' = H) [S24]; 5×10^{-4} (R = H, R' = Et) [S20]; 6×10^{-4}, 3×10^{-4} (R = Br, Cl, resp., R' = Et) [S12,S19]; 3.3×10^{-5}, 7.4×10^{-6} (R = Ph, R' = Me, Et, resp.) [S30]	**E = E' = Se**: 0.17 (R = Me, R' = H) [S24]; 0.17, 0.10 (5 GPa) (R = Cl, R' = Me) [S9]; 0.19, ~0 (7.3 GPa) (R = Cl, R' = Et), 0.23, ~0 (9.4 GPa) (R = Br, R' = Et) [S12,S19]	**E = E' = Se**: T_C = 17.0, 21, 18, 16 (100 kPa, 0.9, 1.6, 2-4 GPa, resp.) (R = Cl, R' = Et); 17.5, 24 (2-4 GPa) (R = Br, R' = Et) [S12,S19,S25-S27]; 10.5, 27.5 (2.4 GPa) (R = I, R' = Et) [S28,S29]; T_N = 27[d] (R = H, R' = Et) [S20]
2 	**E = E' = S**: 10^{-7} (0.5 GPa), 10^{-4} (5 GPa) (R = F, R' = Et; α); 4×10^{-4} (0.5 GPa), 10^{-4} (1.5 GPa) (R = F, R' = Et; β) [S31]	–	–
	**E = Se, E' = S**: 10^{-6} (100 kPa), 10, 1, 10^{-1} (5 GPa) (R = H, F, Me, resp., R' = Me) [S23]; 2.3×10^{-6}, 10^{-1} (4 GPa) (R = H, R' = Me) [S22,S32]; 5.8×10^{-7}, 10^{-2} (4 GPa) (R = H, R' = Et) [S22]	**E = Se, E' = S**: 0.32, ~0 (5-9 GPa) (R = H, R' = Me) [S22,S23,S32]; 0.36 (R = H, R' = Et) [S22]	–

Table S1 *(finished)*

1	2	3	4
	**E = E' = S**: 10^{-4} [S33]	–	–
	**E = E' = S**: 9.7×10^{-4}, 0.2 (5 GPa) (R = Me) [S34]	**E = E' = S**: 0.12 (80-100 K), 0.19 (100-295 K), 0.13 (3-4 GPa), 0.11 (5.5 GPa) (R = Me) [S34]	
	**E = E' = S**: ~10^{-7} (R = Et) [S35]	–	–
	**E = E' = S**: 10^{-3} (M = Al, X = Cl) [S36]	–	**E = E' = S**: (M = Ga, X = Br) [S37] [f]
	**E = E' = S** (BT): 10^{-2} ($[BT]_3[ClO_4]_2$, $[BT]_3[FSO_3]_2$; 10^{-5} ($[BT][ClO_4]$) [S38] **E = Se, E' = S** (BSe): 10^{-1} ($[BSe]_3[ClO_4]_2$) [S39]	–	–
	**E = E' = S** (NT): 10^{-2} ($[NT]_3[BF_4]_2$) [S40]; 0.5 ($[NT]_3[GaCl_4]$); 0.4 ($[NT]_3[FeCl_4]$) [S41,S42]	0.18 ($[NT]_3[GaCl_4]$, $[NT]_3[FeCl_4]$) [S41,S42] [g]	–

[a] σ – electrical conductivity at 295-300 K and ambient pressure (unless otherwise indicated); E_a is thermal activation energy, E_a ~0 means *metallic* conductivity; α and β encode polymorphs.

[b] Curie or Néel temperature T_C and T_N, respectively.

[c] For comparison, for spin-canted AFM (weak FM) 4-R-1,2,3,5-dithiadiazolyl (R = 4-NCC_6F_4) T_N increases from 36 K at normal pressure (~100 kPa) to 70 K at 1.6 GPa [S43,S44].

[d] Spin-canted AFM.

[e] The metamagnet whose magnetic alignment depends on the magnitude of the applied magnetic field and switches from AF to FM with *H* = 6-8 kOe.

[f] Strongly frustrated AF interactions without signs of magnetic order were observed [S37].

[g] Negative differential resistance with threshold field of 80 V cm^{-1} [S41].

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