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Supporting Information

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A theoretical study of the stable radicals galvinoxyl, azagalvinoxyl and Wurster's blue perchlorate in the solid-state

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Table S1. The lattice vectors (in Å) and fractional coordinates of the PBE optimised high-temperature crystal structure of galvinoxyl (**1**).

	X	Y	Z
a	11.8900	5.4350	0.0000
b	11.8900	-5.4350	0.0000
c	-20.7260	0.0000	-10.2445

Atom	a	b	c	Atom	a	b	c	Atom	a	b	c
C	0.7859	0.7141	0.7500	C	0.4687	0.7136	0.7668	H	0.8026	0.4525	0.1686
C	0.6659	0.6967	0.6401	C	0.7864	0.0313	0.7332	H	0.1376	0.0829	0.4530
C	0.8033	0.8341	0.8599	C	0.2920	0.4575	0.6103	H	0.4171	0.3624	0.0470
C	0.7105	0.5757	0.5600	C	0.0425	0.2080	0.8897	H	0.3708	0.0965	0.5757
C	0.9243	0.7895	0.9400	C	0.7850	0.9838	0.4309	H	0.4035	0.1292	0.9243
C	0.6143	0.5533	0.4555	C	0.5162	0.7150	0.0691	H	0.2725	0.9234	0.4082
C	0.9467	0.8857	0.0445	C	0.9307	0.2316	0.6668	H	0.5766	0.2275	0.0918
C	0.4509	0.6546	0.4202	C	0.2684	0.5693	0.8332	H	0.1133	0.3867	0.2500
C	0.8454	0.0491	0.0798	C	0.7437	0.9957	0.5233	H	0.1680	0.4961	0.4112
C	0.4012	0.7777	0.5011	C	0.5043	0.7563	0.9767	H	0.0039	0.3320	0.0888
C	0.7223	0.0988	0.9989	O	0.3553	0.6357	0.3234	H	0.5350	0.1259	0.3412
C	0.5056	0.7907	0.6035	O	0.8643	0.1447	0.1766	H	0.3741	0.9650	0.1588
C	0.7093	0.9944	0.8965	O	0.6447	0.3643	0.6766	H	0.1215	0.7482	0.6314
C	0.6733	0.4320	0.3780	O	0.1357	0.8553	0.8234	H	0.7518	0.3785	0.8686
C	0.0680	0.8267	0.1220	H	0.8867	0.6133	0.7500	H	0.0432	0.5683	0.4693
C	0.2375	0.8890	0.4699	H	0.8320	0.5039	0.5888	H	0.9317	0.4568	0.0307
C	0.6110	0.2625	0.0301	H	0.9961	0.6680	0.9112	H	0.1717	0.7452	0.5782
C	0.8443	0.3385	0.4290	H	0.4650	0.8741	0.6588	H	0.7548	0.3283	0.9218
C	0.1615	0.6557	0.0710	H	0.6259	0.0350	0.8412	H	0.4219	0.7995	0.8197
C	0.5313	0.2864	0.2332	H	0.8785	0.2518	0.3686	H	0.7005	0.0781	0.6803
C	0.2136	0.9687	0.2668	H	0.2482	0.6215	0.1314	H	0.4916	0.7963	0.7770
C	0.7080	0.5425	0.3897	H	0.9568	0.4317	0.5307	H	0.7037	0.0084	0.7230
C	0.9575	0.7920	0.1103	H	0.0683	0.5432	0.9693	H	0.5943	0.6578	0.8121
C	0.2150	0.0162	0.5691	H	0.8283	0.2548	0.4218	H	0.8422	0.9057	0.6879
C	0.4838	0.2850	0.9309	H	0.2452	0.6717	0.0782	H	0.2404	0.5438	0.6603
C	0.0693	0.7684	0.3332	H	0.5781	0.2005	0.1803	H	0.9562	0.2596	0.8397
C	0.7316	0.4307	0.1668	H	0.2995	0.9219	0.3197	H	0.4137	0.3988	0.6550
C	0.2563	0.0043	0.4767	H	0.5084	0.2037	0.2230	H	0.1012	0.0863	0.8450
C	0.4957	0.2437	0.0233	H	0.2963	0.9916	0.2770	H	0.1930	0.3509	0.5074
C	0.2141	0.2859	0.2500	H	0.4057	0.3422	0.1879	H	0.1491	0.3070	0.9926
C	0.3341	0.3033	0.3599	H	0.1578	0.0943	0.3121	H	0.9031	0.9061	0.4568
C	0.1967	0.1659	0.1401	H	0.7596	0.4562	0.3397	H	0.5939	0.5969	0.0432
C	0.2895	0.4243	0.4400	H	0.0438	0.7404	0.1603	H	0.8034	0.0533	0.4299
C	0.0757	0.2105	0.0600	H	0.5863	0.6012	0.3450	H	0.4467	0.6966	0.0701
C	0.3857	0.4467	0.5445	H	0.8988	0.9137	0.1550	H	0.6718	0.8899	0.3314
C	0.0533	0.1143	0.9555	H	0.8070	0.6491	0.4926	H	0.6101	0.8282	0.1686
C	0.5491	0.3454	0.5798	H	0.8509	0.6930	0.0074	H	0.0465	0.1506	0.6908
C	0.1546	0.9509	0.9202	H	0.0969	0.0939	0.5432	H	0.3494	0.4535	0.8092
C	0.5988	0.2223	0.4989	H	0.4061	0.4031	0.9568	H	0.9210	0.3280	0.7420
C	0.2777	0.9012	0.0011	H	0.1966	0.9467	0.5701	H	0.1720	0.5790	0.7580
C	0.4944	0.2093	0.3965	H	0.5533	0.3034	0.9299	H	0.9525	0.3026	0.6686
C	0.2907	0.0056	0.1035	H	0.3282	0.1101	0.6686	H	0.1974	0.5475	0.8314

C	0.3267	0.5680	0.6220	H	0.3899	0.1718	0.8314	H	0.8624	0.9171	0.5470
C	0.9320	0.1733	0.8780	H	0.9535	0.8494	0.3092	H	0.5829	0.6376	0.9530
C	0.7625	0.1110	0.5301	H	0.6506	0.5465	0.1908	H	0.6292	0.9035	0.4243
C	0.3890	0.7375	0.9699	H	0.0790	0.6720	0.2580	H	0.5965	0.8708	0.0757
C	0.1557	0.6615	0.5710	H	0.8280	0.4210	0.2420	H	0.7275	0.0766	0.5918
C	0.8385	0.3443	0.9290	H	0.0475	0.6974	0.3314	H	0.4234	0.7725	0.9082

Table S2. The lattice vectors (in Å) and fractional coordinates of the proposed low-temperature crystal structure of galvinoxyl (**1**).

	X	**Y**	**Z**
a	10.5147	-0.1268	0.0067
b	-1.7173	12.0485	0.1171
c	-0.5222	-2.2378	9.8463

Atom	**a**	**b**	**c**	**Atom**	**a**	**b**	**c**	**Atom**	**a**	**b**	**c**
O	0.4273	0.7758	0.1030	C	0.9020	0.1257	0.6715	H	0.8810	0.9844	0.1264
O	0.1431	0.4702	0.5922	C	0.8938	0.7735	0.8000	H	0.8381	0.0093	0.2959
O	0.5727	0.2242	0.8970	C	0.8538	0.1881	0.9104	H	0.5899	0.5511	0.7640
O	0.8569	0.5298	0.4078	C	0.0306	0.7171	0.6122	H	0.5333	0.6167	0.9184
C	0.4906	0.1779	0.4853	C	0.7956	0.2952	0.7345	H	0.5280	0.4672	0.8793
C	0.4412	0.8661	0.1922	C	0.8956	0.5690	0.7132	H	0.7865	0.0912	0.1819
C	0.2284	0.4107	0.5608	C	0.3176	0.0846	0.8567	H	0.5872	0.2073	0.5373
C	0.3299	0.8998	0.2665	C	0.6203	0.4697	0.2326	H	0.7301	0.9730	0.5828
C	0.2093	0.3211	0.4343	C	0.3550	0.0831	0.0058	H	0.7187	0.8219	0.6743
C	0.3490	0.0005	0.3599	C	0.7191	0.4810	0.1258	H	0.3266	0.9088	0.6427
C	0.2921	0.2445	0.4173	C	0.2816	0.2003	0.8446	H	0.4785	0.6403	0.3171
C	0.4723	0.0714	0.3935	C	0.6257	0.3595	0.2843	H	0.9943	0.1846	0.6922
C	0.4028	0.2535	0.5100	C	0.1969	0.9941	0.8094	H	0.9195	0.0434	0.6911
C	0.5805	0.0354	0.3286	C	0.4842	0.4591	0.1643	H	0.9746	0.7738	0.8728
C	0.4322	0.3513	0.6193	H	0.2699	0.0270	0.4172	H	0.8720	0.1142	0.5633
C	0.5688	0.9409	0.2261	H	0.2813	0.1781	0.3257	H	0.9010	0.8602	0.7813
C	0.3507	0.4286	0.6482	H	0.6734	0.0912	0.3573	H	0.8038	0.7533	0.8475
C	0.1975	0.8240	0.2382	H	0.5215	0.3597	0.6829	H	0.9484	0.2439	0.9287
C	0.0988	0.3157	0.3289	H	0.0057	0.8154	0.3078	H	0.7884	0.2252	0.9812
C	0.0980	0.8743	0.3285	H	0.0805	0.9566	0.3089	H	0.1104	0.7216	0.6885
C	0.1062	0.2265	0.2000	H	0.0254	0.2262	0.1272	H	0.8667	0.1049	0.9308
C	0.1462	0.8119	0.0896	H	0.1280	0.8858	0.4367	H	0.0426	0.6546	0.5213
C	0.9694	0.2829	0.3878	H	0.0990	0.1398	0.2187	H	0.0352	0.8012	0.5868
C	0.2044	0.7048	0.2655	H	0.1962	0.2467	0.1525	H	0.8912	0.3489	0.7605
C	0.1044	0.4310	0.2868	H	0.0516	0.7561	0.0713	H	0.7703	0.2912	0.6266
C	0.6824	0.9154	0.1433	H	0.2116	0.7748	0.0188	H	0.8044	0.5466	0.7579
C	0.3797	0.5303	0.7674	H	0.8896	0.2784	0.3115	H	0.9752	0.5749	0.7905
C	0.6450	0.9169	0.9942	H	0.1333	0.8951	0.0692	H	0.9058	0.5010	0.6275
C	0.2809	0.5190	0.8742	H	0.9574	0.3454	0.4787	H	0.7258	0.3366	0.7952
C	0.7184	0.7997	0.1554	H	0.9648	0.1988	0.4132	H	0.2725	0.0966	0.0661
C	0.3743	0.6405	0.7157	H	0.1088	0.6511	0.2395	H	0.3796	1.0000	0.0133
C	0.8031	0.0059	0.1906	H	0.2297	0.7088	0.3734	H	0.7150	0.5580	0.0858
C	0.5158	0.5409	0.8357	H	0.1956	0.4534	0.2421	H	0.6954	0.4069	0.0410

C	0.5094	0.8221	0.5147	H	0.0248	0.4251	0.2095	H	0.8176	0.4848	0.1691
C	0.5588	0.1339	0.8078	H	0.0942	0.4990	0.3725	H	0.4375	0.1494	0.0492
C	0.7716	0.5893	0.4392	H	0.2742	0.6634	0.2048	H	0.2013	0.2182	0.9069
C	0.6701	0.1002	0.7335	H	0.7275	0.9034	0.9339	H	0.3636	0.2693	0.8776
C	0.7907	0.6789	0.5657	H	0.6204	0.0000	0.9867	H	0.7216	0.3592	0.3313
C	0.6510	0.9995	0.6401	H	0.2850	0.4420	0.9142	H	0.6010	0.2857	0.1991
C	0.7079	0.7555	0.5827	H	0.3046	0.5931	0.9590	H	0.5549	0.3508	0.3594
C	0.5277	0.9286	0.6065	H	0.1824	0.5152	0.8309	H	0.2498	0.1991	0.7390
C	0.5972	0.7465	0.4900	H	0.5625	0.8506	0.9508	H	0.1190	0.0156	0.8736
C	0.4195	0.9646	0.6714	H	0.7987	0.7818	0.0931	H	0.1619	0.9907	0.7041
C	0.5678	0.6487	0.3807	H	0.6364	0.7307	0.1224	H	0.4101	0.4489	0.2360
C	0.4312	0.0591	0.7739	H	0.2784	0.6408	0.6687	H	0.4667	0.3833	0.0816
C	0.6493	0.5714	0.3518	H	0.3990	0.7143	0.8009	H	0.4720	0.5328	0.1207
C	0.8025	0.1760	0.7618	H	0.4451	0.6492	0.6406	H	0.2135	0.9088	0.8181
C	0.9012	0.6843	0.6711	H	0.7502	0.8009	0.2610	H	0.4128	0.7927	0.4627