Investigating Crystal Violet Reactivity and Color with Quantum Theory and Interactive Webpages

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Cartesian coordinates of ions and molecules

All optimized at the B3LYP/6-31G(d,p)/SMD-water level of theory with ORCA-6.0 .

To copy these coordinates for inserting into WebMO or other computational programs,
first convert the PDF into an Excel worksheet using Adobe Acrobat, PDFCandy,
or an online PDF-to-Excel converter.

		x	y	z
Crystal violet	C	0.0000	0.0000	0.0000
	N	-0.3408	1.2850	-0.6107
	C	0.7056	2.0400	-1.2996
	H	0.5309	2.0815	-2.3817
	H	0.7705	3.0651	-0.9197
	H	1.6645	1.5537	-1.1257
	C	-1.6272	1.7288	-0.6112
	C	-2.6629	1.0054	0.0513
	C	-3.9653	1.4563	0.0361
	C	-4.3413	2.6667	-0.6097
	C	-3.2988	3.3875	-1.2557
	C	-1.9963	2.9370	-1.2735
	H	-1.2540	3.5069	-1.8181
	H	-3.5407	4.2941	-1.8002
	C	-5.7094	3.1356	-0.6146
	C	-6.7988	2.1844	-0.6137
	C	-8.0414	2.4665	0.0189
	C	-9.0808	1.5613	0.0325
	C	-8.9626	0.2969	-0.6170
	C	-7.7257	0.0103	-1.2670
	C	-6.6874	0.9166	-1.2489
	H	-5.7763	0.6715	-1.7843
	H	-7.5966	-0.9212	-1.8036
	N	-9.9876	-0.5982	-0.6157
	C	-11.2800	-0.2437	-0.0283
	H	-11.7090	0.6432	-0.5087
	H	-11.9710	-1.0743	-0.1654
	H	-11.1910	-0.0468	1.0462
	C	-9.8458	-1.8912	-1.2848
	H	-8.9899	-2.4492	-0.8908
	H	-10.7440	-2.4807	-1.1075
	H	-9.7168	-1.7765	-2.3681
	H	-9.9900	1.8171	0.5619
	H	-8.1632	3.4032	0.5525
	C	-5.9878	4.5546	-0.6232
	C	-7.1369	5.0896	-1.2688
	C	-7.4028	6.4418	-1.2931
	C	-6.5407	7.3721	-0.6402
	C	-5.3928	6.8444	0.0220
	C	-5.1274	5.4919	0.0131
	H	-4.2604	5.1303	0.5558
	H	-4.7225	7.5052	0.5574

		x	y	z
Crystal violet alcohol	C	0.0000	0.0000	0.0000
	C	-1.0923	-0.9885	-0.4420
	C	-2.3310	-0.9925	0.2182
	C	-3.3623	-1.8467	-0.1577
	C	-3.2073	-2.7551	-1.2326
	N	-4.2231	-3.6537	-1.5846
	C	-5.5859	-3.3251	-1.1644
	H	-5.6631	-3.2846	-0.0752
	H	-5.9413	-2.3662	-1.5726
	H	-6.2578	-4.1141	-1.5067
	C	-4.1428	-4.2661	-2.9107
	H	-3.2358	-4.8680	-3.0100
	H	-4.9934	-4.9377	-3.0393
	H	-4.1582	-3.5269	-3.7267
	C	-1.9688	-2.7318	-1.9101
	C	-0.9412	-1.8739	-1.5134
	H	-0.0069	-1.9009	-2.0654
	H	-1.7910	-3.3880	-2.7533
	H	-4.2942	-1.8005	0.3930
	H	-2.4995	-0.3089	1.0451
	C	-0.3844	1.4311	-0.4286
	C	-0.2049	2.5257	0.4252
	C	-0.5333	3.8252	0.0394
	C	-1.0733	4.0980	-1.2374
	C	-1.2391	2.9933	-2.1048
	C	-0.9105	1.7016	-1.7002
	H	-1.0712	0.8867	-2.4005
	H	-1.6379	3.1323	-3.1024
	N	-1.4642	5.3908	-1.6122
	C	-0.9139	6.5069	-0.8428
	H	-1.2168	6.4478	0.2057
	H	0.1854	6.5567	-0.8833
	H	-1.3146	7.4401	-1.2428
	C	-1.5915	5.6628	-3.0445
	H	-2.3598	5.0314	-3.4975
	H	-1.9053	6.6995	-3.1785
	H	-0.6501	5.5121	-3.5954
	H	-0.3691	4.6263	0.7497
	H	0.1934	2.3759	1.4240
	C	1.3938	-0.4101	-0.5087
	C	2.0700	0.2332	-1.5513
	C	3.3306	-0.1839	-1.9804

	N	-6.8030	8.7071	-0.6494
	C	-8.0211	9.2187	-1.2776
	H	-8.9192	8.7892	-0.8191
	H	-8.0570	10.3000	-1.1514
	H	-8.0417	8.9990	-2.3512
	C	-5.8991	9.6457	0.0155
	H	-4.8837	9.5743	-0.3893
	H	-6.2593	10.6600	-0.1487
	H	-5.8547	9.4674	1.0967
	H	-8.2728	6.7939	-1.8330
	H	-7.8027	4.4211	-1.8041
	H	-4.7154	0.8912	0.5791
	H	-2.4315	0.0959	0.5916
	H	-0.2129	-0.0019	1.0750
	H	-0.5538	-0.8244	-0.4640
	H	1.0648	-0.1845	-0.1354
OH-4-water	O	0.0000	0.0000	0.0000
cluster	H	0.7127	-0.6792	-0.0007
	H	-0.4618	-0.1736	0.8515
	O	1.3452	-1.5073	2.7315
	H	1.7689	-1.8602	3.5246
	H	1.8994	-1.7604	1.3263
	O	2.1761	-1.7554	0.3372
	H	2.7710	-0.9925	0.2996
	O	1.8668	1.0084	2.0397
	H	1.2856	0.9409	1.2607
	H	1.7674	0.0842	2.4156
	O	-0.9629	-0.4350	2.6188
	H	-0.0757	-0.9329	2.7593
	H	-0.7157	0.4746	2.8399
CV-OH	C	0.0000	0.0000	0.0000
4-water	N	1.0596	-0.9891	-0.1964
transition state	C	2.3565	-0.6633	0.1364
	C	2.6521	0.4689	0.9453
	C	3.9531	0.7731	1.3028
	C	5.0499	-0.0236	0.8989
	C	6.4283	0.3226	1.2809
	C	6.8568	1.7269	1.1572
	C	7.9693	2.2247	1.8749
	C	8.4031	3.5316	1.7483
	C	7.7467	4.4431	0.8755
	C	6.6472	3.9412	0.1335
	C	6.2150	2.6315	0.2858
	H	5.3817	2.2933	-0.3201
	H	6.1304	4.5747	-0.5764
	N	8.1537	5.7559	0.7708
	C	9.4603	6.1437	1.3021
	H	9.5197	5.9562	2.3779
	H	10.2877	5.6124	0.8108
	H	9.5990	7.2141	1.1478
	C	7.6131	6.5862	-0.3042
	H	6.5225	6.6389	-0.2470
	C	3.9823	-1.2873	-1.3861
	C	3.3047	-1.9262	-0.3200
	C	2.0473	-1.4985	0.0928
	H	1.5658	-2.0207	0.9142
	H	3.7565	-2.7654	0.1950
	N	5.2205	-1.7479	-1.8478
	C	6.0214	-0.8310	-2.6588
	H	5.4925	-0.5520	-3.5734
	H	6.2944	0.0906	-2.1215
	H	6.9400	-1.3392	-2.9573
	C	6.0092	-2.5867	-0.9447
	H	5.4747	-3.5064	-0.6946
	H	6.9311	-2.8760	-1.4522
	H	6.2760	-2.0747	-0.0072
	H	3.8035	0.3659	-2.7851
	H	1.6201	1.0880	-2.0454
	O	0.0081	-0.0858	1.4476
	H	0.8209	0.3431	1.7550
Crystal violet	C	0.0000	0.0000	0.0000
alcohol-4-	N	1.2348	-0.7618	-0.1905
water cluster	C	2.3807	-0.3102	0.4745
	C	3.6748	-0.7198	0.0841
	C	4.8069	-0.3210	0.7956
	C	4.7189	0.5175	1.9117
	C	5.9481	1.0084	2.6883
	C	7.1934	0.1457	2.4364
	C	7.2264	-1.1802	2.9036
	H	6.3699	-1.5836	3.4355
	C	8.3342	-1.9986	2.7153
	H	8.3002	-3.0068	3.1098
	C	9.4806	-1.5355	2.0246
	C	9.4477	-0.2004	1.5646
	C	8.3301	0.6094	1.7653
	H	8.3624	1.6273	1.3916
	H	10.2996	0.2238	1.0471
	N	10.5766	-2.3702	1.7830
	C	10.7306	-3.5479	2.6384
	H	9.8775	-4.2228	2.5377
	H	10.8466	-3.2910	3.7026
	H	11.6176	-4.0985	2.3196
	C	11.8396	-1.7328	1.4130
	H	11.7366	-1.1679	0.4832
	H	12.5866	-2.5094	1.2389
	H	12.2206	-1.0532	2.1909
	C	6.2001	2.5015	2.4158
	C	6.0304	3.0475	1.1361
	C	6.3009	4.3863	0.8628
	C	6.7456	5.2662	1.8763
	C	6.9303	4.7101	3.1626
	C	6.6624	3.3661	3.4165
	H	6.8165	3.0006	4.4270
	H	7.2819	5.3251	3.9819
	N	6.9564	6.6277	1.6270
	C	7.7899	7.3631	2.5784

H	7.9973	7.6006	-0.1925
H	7.8912	6.2174	-1.3019
H	9.2524	3.8542	2.3376
H	8.4885	1.5708	2.5680
C	7.4599	-0.7287	1.2160
C	8.7070	-0.5099	0.5925
C	9.6625	-1.5093	0.4838
C	9.4300	-2.8081	1.0049
C	8.1835	-3.0263	1.6543
C	7.2340	-2.0240	1.7396
H	6.3066	-2.2306	2.2628
H	7.9628	-3.9864	2.1038
N	10.3597	-3.8160	0.8731
C	11.7227	-3.4807	0.4638
H	11.7307	-2.9946	-0.5159
H	12.2257	-2.8190	1.1830
H	12.3017	-4.4007	0.3787
C	10.1867	-5.0562	1.6281
H	9.2333	-5.5331	1.3860
H	10.9817	-5.7495	1.3499
H	10.2307	-4.8973	2.7150
H	10.5937	-1.2796	-0.0194
H	8.9253	0.4577	0.1546
C	4.7532	-1.1407	0.0904
C	3.4566	-1.4481	-0.2950
H	3.3006	-2.3002	-0.9445
H	5.5596	-1.7634	-0.2810
H	4.1277	1.6343	1.9387
H	1.8547	1.1089	1.3023
C	0.8184	-2.0129	-1.2118
H	1.2772	-2.9633	-0.9253
H	-0.2562	-2.1783	-1.2961
H	1.2042	-1.7250	-2.2002
H	-0.0821	0.2865	1.0523
H	0.1594	0.9093	-0.5964
H	-0.9518	-0.4426	-0.2946
O	2.9323	0.6731	5.0040
H	3.5362	1.3833	4.6925
H	3.2495	-0.1162	4.5135
O	6.1141	0.2869	3.4007
H	7.0233	0.0790	3.6622
H	5.5098	1.6975	3.9794
O	5.0196	2.4802	4.3787
H	5.2453	2.4125	5.3183
O	5.3915	0.0547	6.3819
H	4.4632	0.2468	6.1414
H	5.8207	0.0956	5.5085
O	4.3018	-1.5570	3.9128
H	5.0297	-0.8998	3.6784
H	4.5263	-1.7937	4.8254

H	7.3448	7.3573	3.5764
H	7.8527	8.4043	2.2577
H	8.8122	6.9610	2.6528
C	7.1441	7.0350	0.2342
H	7.2797	8.1175	0.2010
H	8.0193	6.5616	-0.2374
H	6.2614	6.8009	-0.3658
H	6.1536	4.7429	-0.1493
H	5.6838	2.4163	0.3232
O	5.5887	0.8439	4.1060
H	6.4093	0.8639	4.6235
C	3.4372	0.9569	2.2799
C	2.2973	0.5557	1.5914
H	1.3375	0.9254	1.9306
H	3.3197	1.6345	3.1197
H	5.7766	-0.6714	0.4574
H	3.8118	-1.3623	-0.7770
C	1.4081	-1.2837	-1.5465
H	1.8302	-0.5403	-2.2402
H	0.4354	-1.5973	-1.9294
H	2.0563	-2.1635	-1.5494
H	-0.2951	0.0116	1.0519
H	-0.8025	-0.4885	-0.5555
H	0.0797	1.0411	-0.3492
O	1.9421	0.2949	5.6013
H	2.4076	1.1417	5.4459
H	2.5994	-0.3638	5.2813
H	4.4636	1.9877	5.1185
O	3.8455	2.4603	5.7103
H	3.9132	1.9603	6.5506
O	3.5838	0.6044	7.8647
H	4.3062	0.0095	7.6159
H	2.8704	0.3603	7.2344
O	4.0774	-1.3842	4.9181
H	4.3882	-1.5537	5.8197
H	4.6282	-0.6278	4.6191

		x	y	z
4IV	O	0.0098	0.0437	-0.0556
	H	0.8196	-0.1142	-0.6179

		x	y	z
4I	O	-0.0023	-0.0007	0.0010
	H	-0.6109	0.7433	-0.3791

	H	0.4454	0.0830	0.8136
	O	0.5822	-2.6947	-0.9463
	H	0.0209	-2.0792	-0.4435
	O	2.3736	-0.7148	-1.0199
	H	2.8674	-0.3598	-1.7712
	H	1.3086	-2.0595	-1.1973
	O	3.0522	-2.6814	0.6486
	H	2.1618	-3.0414	0.4948
	H	3.0363	-1.9516	-0.0322
	O	2.4796	0.0769	1.5204
	H	2.5739	-0.8625	1.7536
	H	2.5505	-0.0077	0.5274
4III	O	0.0016	-0.0010	-0.0035
	H	-0.5883	0.6667	-0.5125
	H	0.2273	0.4740	0.8087
	O	-3.7709	1.1218	0.0061
	H	-3.6842	1.6326	0.8233
	O	-1.5766	1.6240	-1.2462
	H	-1.7184	1.1573	-2.0824
	H	-2.9114	1.3534	-0.5110
	O	-2.3792	-1.1011	1.0281
	H	-2.9618	-0.3861	0.6904
	H	-1.5009	-0.8153	0.6946
	O	-1.2760	4.0995	-2.1259
	H	-2.1723	4.3238	-2.4086
	H	-1.3766	3.1578	-1.7838
4II-up	O	0.0140	-0.0456	-0.0139
	H	-0.6114	0.5887	-0.5236
	H	0.4065	0.5478	0.6428
	O	-3.9708	0.9667	0.0060
	H	-4.0331	1.6787	0.6593
	O	-1.7087	1.5448	-1.0188
	H	-1.5557	2.1677	-1.7408
	H	-3.1222	1.2283	-0.5092
	O	-2.1907	-0.3992	1.7193
	H	-2.8938	-0.0386	1.1324
	H	-1.4054	-0.4130	1.1264
	O	-1.4749	2.4557	1.4665
	H	-1.6950	1.5819	1.8365
	H	-1.5271	2.2491	0.4857

	H	-0.2366	-0.7771	-0.5265
	O	-3.7168	0.4118	-0.2616
	H	-3.5940	-0.4002	-0.7727
	O	-1.6392	1.8001	-0.7329
	H	-1.5414	2.2395	-1.5875
	H	-2.9123	0.9992	-0.5404
	O	-2.0524	-0.2785	1.8858
	H	-2.7504	-0.0943	1.2144
	H	-1.2407	-0.2495	1.3264
	O	-1.8214	2.6211	1.7817
	H	-1.9031	1.6894	2.0606
	H	-1.7399	2.4996	0.7962
4II	O	-0.0131	0.1516	0.1885
	H	-0.6654	0.7642	-0.3174
	H	0.3356	0.7637	0.8534
	O	-3.9194	0.5629	-0.1578
	H	-3.8942	-0.2698	-0.6498
	O	-1.7606	1.7421	-0.7816
	H	-1.6325	2.2233	-1.6091
	H	-3.0895	1.0720	-0.5028
	O	-2.2175	-0.2304	1.9189
	H	-2.9124	0.0137	1.2628
	H	-1.4128	-0.2580	1.3542
	O	-1.3690	2.5696	1.7054
	H	-1.6793	1.7061	2.0363
	H	-1.4986	2.4335	0.7232