The structure of oxotitanium phthalocyanine: a gas-phase electron diffraction and computational study

Alexander V. Zakharov,* Sergei A. Shlykov,

Yuriy A. Zhabanov and Georgy V. Girichev

Department of Physics, Ivanovo State University of Chemistry and Technology
Engelsa 7, Ivanovo, 153000, Russian Federation. E-mail: a_zakharov@isuct.ru

Supplementary information

Cartesian coordinates of the experimental (r_{h1}) structure of oxotitanium phthalocyanine (in Å).

Ti1	0.0000	0.0000	0.0000
O2	0.0000	0.0000	1.6001
N3	1.9944	0.0000	-0.6270
N4	0.0000	1.9944	-0.6270
N5	-1.9944	0.0000	-0.6270
N6	0.0000	-1.9944	-0.6270
N7	2.3811	-2.3811	-0.7747
N8	2.3811	2.3811	-0.7747
N9	-2.3811	2.3811	-0.7747
N10	-2.3811	-2.3811	-0.7747
C11	2.7862	-1.1243	-0.7216
C12	1.1243	2.7862	-0.7216
C13	-2.7862	1.1243	-0.7216
C14	-1.1243	2.7862	-0.7216
C15	-2.7862	-1.1243	-0.7216
C16	1.1243	-2.7862	-0.7216
C17	2.7862	1.1243	-0.7216
C18	-1.1243	-2.7862	-0.7216
C19	4.1814	-0.7098	-0.8274
C20	0.7098	4.1814	-0.8274
C21	-4.1814	0.7098	-0.8274
C22	-0.7098	4.1814	-0.8274
C23	-4.1814	-0.7098	-0.8274
C24	0.7098	-4.1814	-0.8274
C25	4.1814	0.7098	-0.8274
C26	-0.7098	-4.1814	-0.8274
C27	5.3704	-1.4277	-0.9433

C28	1.4277	5.3704	-0.9433
C29	-5.3704	1.4277	-0.9433
C30	-1.4277	5.3704	-0.9433
C31	-5.3704	-1.4277	-0.9433
C31	-5.3704	-1.4277	-0.9433
C32	1.4277	-5.3704	-0.9433
C33	5.3704	1.4277	-0.9433
C34	-1.4277	-5.3704	-0.9433
C35	6.5622	-0.7166	-1.0358
C36	0.7166	6.5622	-1.0358
C37	-6.5622	0.7166	-1.0358
C38	-0.7166	6.5622	-1.0358
C39	-6.5622	-0.7166	-1.0358
C40	0.7166	-6.5622	-1.0358
C41	6.5622	0.7166	-1.0358
C42	-0.7166	-6.5622	-1.0358
H43	5.4029	-2.4925	-0.9609
H44	2.4925	5.4029	-0.9609
H45	-5.4029	2.4925	-0.9609
H46	-2.4925	5.4029	-0.9609
H47	-5.4029	-2.4925	-0.9609
H48	2.4925	-5.4029	-0.9609
H49	5.4029	2.4925	-0.9609
H50	-2.4925	-5.4029	-0.9609
H51	7.5337	-1.1483	-1.1224
H52	1.1483	7.5337	-1.1224
H53	-7.5337	1.1483	-1.1224
H54	-1.1483	7.5337	-1.1224
H55	-7.5337	-1.1483	-1.1224
H56	1.1483	-7.5337	-1.1224
H57	7.5337	1.1483	-1.1224
H58	-1.1483	-7.5337	-1.1224

List of experimental distances (r_a), r.m.s. vibrational amplitudes (l_a) and vibrational corrections (k_{h1}).

Distance	Mult.*	r_a, Å	l_a, Å	k_{h1}, Å
C27-H43	8	1.0647	0.0504	0.00081
C35-H51	8	1.0659	0.0506	0.00068
N7-C11	8	1.3228	0.0492	-0.00126
N3-C11	8	1.3771	0.0545	0.00128
C27-C35	8	1.3912	0.0502	-0.00024
C19-C27	8	1.3936	0.0503	0.00016
C35-C41	4	1.4337	0.0516	-0.00058
C19-C25	4	1.4191	0.0512	0.00047

*Multiplicity, *i.e.* number of symmetrically equivalent distances of this type

C11-C19	8	1.4598	0.0555	-0.00046
Ti1-O2	1	1.6003	0.0449	-0.00023
Ti1-N3	4	2.0898	0.0878	0.00076
C27-H51	8	2.1800	0.1935	0.00859
C35-H57	8	2.0958	0.1944	0.00869
C19-H43	8	2.1566	0.1938	0.00861
C35-H43	8	2.1141	0.1940	0.00805
C11-C17	4	2.2419	0.0717	0.00668
C11-C25	8	2.3028	0.0731	0.00403
N3-C19	8	2.3070	0.0720	0.00105
C11-C16	4	2.3442	0.0740	0.00612
C19-C35	8	2.3835	0.0763	0.00640
N3-N7	8	2.4109	0.0782	0.00587
C27-C41	8	2.4518	0.0769	0.00314
C19-C33	8	2.4445	0.0776	0.00413
N7-C19	8	2.4547	0.0842	0.00240
H51-H57	4	2.2808	0.2649	0.01567
H43-H51	8	2.5105	0.2655	0.01410
C11-C27	8	2.6050	0.0896	0.00644
C19-C41	8	2.7747	0.0883	0.00851
N3-N4	4	2.8099	0.1065	0.01056
C27-C33	4	2.8513	0.0800	0.00407
N3-C12	8	2.9069	0.0928	0.01348
C11-H43	8	2.9495	0.1604	0.01303
N7-H43	8	3.0245	0.2144	0.00510
O2-N3	4	2.9835	0.1670	0.00603
Ti1-C11	8	3.0756	0.1002	0.01425
N7-C27	8	3.1346	0.1268	0.00764
C19-H51	8	3.3755	0.0974	0.01822
C27-H57	8	3.3524	0.0990	0.01617
C19-H49	8	3.4128	0.0987	0.01711
C35-H49	8	3.3973	0.0986	0.01560
Ti1-N7	4	3.4406	0.1042	0.01470
N7-C17	8	3.5154	0.0667	0.01364
N7-C25	8	3.5664	0.0679	0.01098
C11-C33	8	3.6264	0.0671	0.01224
N3-C27	8	3.6675	0.0707	0.01159
C11-C24	8	3.6840	0.0768	0.01317
C11-C35	8	3.7956	0.0778	0.01536
O2-C11	8	3.7726	0.2220	0.02432
C19-H57	8	3.8214	0.1015	0.02269
C27-H49	8	3.9014	0.1006	0.01896
N3-N 5	2	3.9714	0.0951	0.01732
H43-H48	4	4.1891	0.3497	-0.07324
O2-N 7	4	4.0940	0.2591	0.02651
N3-C14	8	4.1582	0.1202	0.02482
C11-C41	8	4.1942	0.0966	0.01844

N3-H43	8	4.2131	0.1603	0.02271
C11-C12	8	4.2249	0.1017	0.02403
C11-H48	8	4.2804	0.2353	0.01492
H43-H57	8	4.1921	0.1528	0.02946
Ti1-C19	8	4.2968	0.1182	0.02443
N3-C20	8	4.3529	0.1122	0.02595
C11-C32	8	4.4431	0.1418	0.02053
C11-H49	8	4.4439	0.1341	0.02660
N7-C35	8	4.4884	0.1359	0.01949
C11-C26	8	4.6219	0.0954	0.02342
N3-C35	8	4.6211	0.0911	0.02071
C11-H51	8	4.7356	0.1248	0.02888
N7-N 8	4	4.7398	0.0841	0.02235
N7-C33	8	4.8233	0.0898	0.02134
C27-H48	8	4.9319	0.2885	-0.02429
N3-C13	8	4.8816	0.1112	0.03025
C19-C24	4	4.8904	0.1054	0.01921
O2-C19	8	4.8471	0.2878	0.03975
C19-H48	8	4.9865	0.2504	0.00301
N3-C22	8	4.9518	0.1077	0.03185
N3-N 9	8	4.9550	0.1171	0.02850
H43-H49	4	4.9483	0.1325	0.03674
N7-C41	8	5.1837	0.1157	0.02642
N7-H51	8	5.2789	0.1852	0.03061
C11-H57	8	5.2429	0.1293	0.03576
N7-C12	8	5.2859	0.1161	0.03228
N3-H44	8	5.3953	0.2366	0.04082
N3-C28	8	5.3691	0.1490	0.04037
C19-C32	8	5.3937	0.1743	0.02087
C11-C14	4	5.4894	0.1316	0.04078
C11-C15	4	5.5329	0.1225	0.03950
C27-C32	4	5.5658	0.2298	0.01004
Ti1-C27	8	5.5950	0.1433	0.04148
N3-H51	8	5.6408	0.1296	0.03797
C11-C20	8	5.6601	0.1204	0.03846
N7-H49	8	5.6982	0.1421	0.03920
C11-C40	8	5.7907	0.1466	0.03622
C11-C34	8	5.9484	0.1101	0.03788
C19-C20	8	5.9628	0.1190	0.03521
Ti1-H43	8	5.9764	0.2162	0.05079
C11-C13	4	5.9624	0.1344	0.04656
O2-C27	8	6.0515	0.3478	0.05979
C35-H48	8	6.2162	0.3122	-0.00897
N3-C21	8	6.1748	0.1235	0.04484
N7-C13	8	6.1983	0.1351	0.04598
N7-H57	8	6.2090	0.1491	0.04616
C19-H44	8	6.3142	0.2582	0.02894

C11-C22	8	6.3070	0.1208	0.04785
N3-C30	8	6.3258	0.1254	0.05009
C11-C42	8	6.4314	0.1265	0.04465
O2-H43	8	6.4083	0.3914	0.06952
H43-H56	8	6.6170	0.3569	-0.01839
C11-H44	8	6.4902	0.2443	0.04794
C11-H56	8	6.5784	0.1899	0.04914
C11-C28	8	6.5863	0.1533	0.05264
C19-C28	8	6.6327	0.1664	0.04307
Ti1-C35	8	6.6257	0.1410	0.05628
N3-C36	8	6.6403	0.1420	0.05763
N7-N9	2	6.6858	0.1432	0.04881
N7-C20	8	6.7222	0.1243	0.04999
C11-H50	8	6.7423	0.1538	0.05683
C19-C40	8	6.7645	0.1768	0.03992
C19-C22	4	6.8674	0.1163	0.04986
C27-C40	8	6.9013	0.2417	0.02915
C11-C23	8	6.9230	0.1282	0.05770
N3-H46	8	6.9655	0.1844	0.06549
N3-C38	8	7.0495	0.1338	0.06245
O2-C35	8	7.0320	0.3785	0.07605
C11-C21	8	7.1442	0.1318	0.06155
N7-C21	8	7.1965	0.1316	0.05761
C35-H44	8	7.3292	0.3009	0.02035
C19-C34	8	7.2426	0.1281	0.05103
C27-H56	8	7.3964	0.2982	0.02941
C27-H44	8	7.3773	0.2756	0.03477
C19-H56	8	7.4245	0.2322	0.04903
N3-C29	8	7.4421	0.1455	0.06647
C11-H58	8	7.4641	0.1627	0.06729
N3-H52	8	7.5216	0.1932	0.07564
C19-C42	8	7.5801	0.1682	0.05441
Ti1-H51	8	7.6252	0.1822	0.07773
C11-C30	8	7.6759	0.1432	0.06916
N7-H44	8	7.7205	0.2580	0.06643
N3-H45	8	7.7382	0.2369	0.07484
N7-C28	8	7.7431	0.1694	0.06854
C27-C28	8	7.8025	0.1981	0.05616
C27-C42	8	7.9122	0.2334	0.05167
C11-C36	8	7.8927	0.1649	0.07373
C19-C36	8	7.9929	0.1831	0.06506
O2-H51	8	7.9941	0.4257	0.09834
C19-H50	8	8.0855	0.1765	0.07440
C11-C31	8	8.0858	0.1676	0.07941
N3-H54	8	8.0914	0.1690	0.08648
C19-C30	8	8.2029	0.1463	0.07022
C11-H47	8	8.2234	0.2578	0.08261

H43-H58	8	8.2276	0.3404	0.04030
C35-C40	4	8.2160	0.2819	0.05102
C19-C23	4	8.2837	0.1568	0.07921
H43-H44	8	8.3495	0.3032	0.06520
C11-H46	8	8.3110	0.2090	0.08702
C11-C38	8	8.3712	0.1597	0.08165
C19-C21	4	8.4011	0.1575	0.08139
C11-C29	8	8.4632	0.1683	0.08617
N3-C37	8	8.5107	0.1614	0.08559
C35-H56	8	8.6557	0.3460	0.05017
N7-C29	8	8.5563	0.1640	0.08202
C19-H58	8	8.5845	0.2007	0.07909
C19-H52	8	8.7103	0.2438	0.07844
C19-C38	8	8.6921	0.1702	0.07809
C11-H52	8	8.7288	0.2164	0.09191
C27-H50	8	8.7265	0.2227	0.08421
H51-H56	4	8.9885	0.4120	0.04187
C11-H45	8	8.8573	0.2427	0.09808
C27-H58	8	8.8582	0.2669	0.07542
C19-H46	8	8.9586	0.1815	0.09264
N7-C36	8	9.0087	0.1637	0.09187
N7-H45	8	9.0876	0.2171	0.09803
C27-C36	8	9.1654	0.2021	0.08146
C35-C36	8	9.2588	0.2452	0.07675
C11-C39	8	9.2604	0.1612	0.10213
N7-C37	8	9.3698	0.1572	0.09830
C11-C37	8	9.4278	0.1582	0.10533
C11-H54	8	9.4099	0.1719	0.10861
C19-C31	8	9.4745	0.1740	0.10498
N3-H53	8	9.4991	0.1804	0.11066
C27-C30	4	9.5209	0.1509	0.09305
C19-H47	8	9.6401	0.2556	0.10956
C35-H52	8	9.7866	0.3102	0.08187
C19-C29	8	9.6798	0.1699	0.10894
C19-H54	8	9.7152	0.1838	0.10554
C27-H52	8	9.8150	0.2629	0.09285
N7-H52	8	9.8835	0.2070	0.11366
C27-C38	8	9.9456	0.1807	0.09922
C19-H45	8	9.9874	0.2461	0.11861
C35-H50	8	10.0836	0.2051	0.11223
C35-C38	4	10.1939	0.2055	0.09992
C11-H55	8	10.2009	0.1833	0.12684
C35-H58	8	10.1894	0.2619	0.10290
C27-H46	8	10.2965	0.1792	0.11900
N7-H53	8	10.4028	0.1693	0.12713
C11-H53	8	10.4413	0.1731	0.13344
H43-H47	4	10.6756	0.3368	0.13019

C19-C39	12	10.6146	0.1735	0.13114
H51-H52	8	10.6705	0.3294	0.10686
C27-H47	8	10.6914	0.2718	0.13440
C19-C37	8	10.7077	0.1611	0.13221
H43-H52	8	10.7657	0.2588	0.12706
C35-H46	8	10.8000	0.1934	0.12893
C27-H54	8	10.9539	0.1947	0.12904
C27-C29	4	10.9737	0.1797	0.14018
H43-H46	4	11.0218	0.2251	0.14403
C35-H54	8	11.1636	0.2372	0.12915
C27-H45	8	11.3129	0.2922	0.15147
C19-H55	8	11.5686	0.2464	0.15847
H43-H45	4	11.7330	0.3366	0.16725
C19-H53	8	11.7029	0.2400	0.16236
C27-C39	8	11.7922	0.2455	0.16196
H43-H54	8	11.8168	0.2651	0.16105
C35-H47	8	11.9305	0.3216	0.16597
C27-C37	8	11.9586	0.2385	0.16554
C35-H45	8	12.2141	0.3097	0.17413
H51-H54	4	12.1179	0.3157	0.16023
C27-H55	8	12.7169	0.2561	0.19145
H43-H55	8	12.8143	0.3282	0.19301
C35-C39	4	12.9314	0.2265	0.19303
C27-H53	8	12.9611	0.2408	0.19887
C35-C37	4	13.0077	0.2230	0.19475
H43-H53	8	13.2310	0.3033	0.20914
C35-H55	8	13.8770	0.2842	0.22586
C35-H53	8	13.9896	0.2769	0.22943
H51-H55	4	14.8078	0.3254	0.25967
H51-H53	4	14.9747	0.3112	0.26676

Correlation coefficients that are larger than 0.5.

Parameters	Coefficient
α(O-Ti-N)/α(Ti-N-C_{p1})	0.51
r(Ti$\cdots$$N_m$)/$\alpha$($C_{p1}$-$C_{p2}$-$C_{b1}$)	0.51
r(Ti-N)/α(O-Ti-N)	0.52
r(Ti$\cdots$$N_m$)/$\alpha$(N-$C_{p1}$-$C_{p2}$)	0.52
r(N-C_{p1})/α(O-Ti-N)	0.53
α(O-Ti-N)/γ(O-Ti-N-C_{p1})	0.54
α(O-Ti$\cdots$$N_m$)/$\alpha$($C_{p1}$-$C_{p2}$-$C_{b1}$)	0.54
r(C_{p2}-C_{b1})/α(C_{p1}-C_{p2}-C_{b1})	0.61
α(N-C_{p1}-C_{p2})/r(C_{b1}-H_{b1})	0.64
α(N-C_{p1}-C_{p2})/r(C_{p2}-C_{b1})	0.66
r(C_{p1}-N)/α(C_{p1}-C_{p2}-C_{b1})	0.66
r(C_{p1}-N)/α(N-C_{p1}-C_{p2})	0.67
α(C_{p1}-C_{p2}-C_{b1})/r(C_{b1}-H_{b1})	0.72
r(C_{p2}-C_{b1})/α(C_{p2}-C_{b1}-C_{b2})	0.88
r(Ti$\cdots$$N_m$)/$\alpha$(O-Ti$\cdots$$N_m$)	0.91
α(N-C_{p1}-C_{p2})/γ(Ti-N-C_{p1}-C_{p2})	0.91
α(N-C_{p1}-C_{p2})/α(C_{p1}-C_{p2}-C_{b1})	0.92