Electronic Supplementary Material (ESI) for Analyst

A Fluorescent Probe Directly Detect Peroxynitrite Based on Boronate Oxidation and Its Applications for Fluorescence Imaging in Living Cells

Fabiao Yu,[a] Ping Song,[b] Peng Li,[b] Bingshuai Wang,[b] and Keli Han*[b]

[a]School of Chemical Engineering, Dalian University of Technology, Dalian, 116024, P. R. China; E-mail: yufabiao@163.com
[b]State Key Laboratory of Moleclar Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences; E-mail: klhan@dicp.ac.cn

XYZ Coordinates (angstrom) and SCF Energies (a.u.)

Py-Bor

Energy = -1026.0453855

C	-1.925781	-5.365063	0.227249
C	-0.571041	-5.508075	-0.023663
C	0.255787	-4.389950	-0.136723
C	-0.305473	-3.095193	0.006633
C	-1.692122	-2.960743	0.262829
C	-2.482837	-4.105718	0.369354
C	1.657377	-4.507963	-0.394257
C	0.516070	-1.940151	-0.102432
C	1.902893	-2.096829	-0.355697
C	2.442260	-3.413421	-0.498215
C	2.703353	-0.959544	-0.452931
H	3.765342	-1.076578	-0.644239

C	2.153428	0.297184	-0.305170
C	0.790090	0.496140	-0.063821
C	-0.043001	-0.639757	0.038730
C	-1.450363	-0.546978	0.297927
C	-2.230131	-1.646276	0.402507
H	-3.293255	-1.547213	0.599670
H	-1.887670	0.436511	0.409327
H	2.076860	-5.503186	-0.503699
H	-2.553265	-6.244930	0.312197
H	-0.134684	-6.495606	-0.135418
H	-3.544339	-3.993952	0.566214
H	3.505829	-3.510049	-0.692344
H	2.801351	1.163863	-0.380254
B	0.310312	1.972592	0.063905
O	-0.984928	2.403151	0.202333
O	1.205809	3.013840	0.036095
C	0.483286	4.212324	0.416930
C	-0.978659	3.846993	0.037601
C	1.050532	5.394457	-0.330410
H	0.444205	6.283707	-0.136727
H	2.067067	5.594397	0.015766
H	1.080626	5.220295	-1.406202
C	0.687948	4.394818	1.909748
H	1.759512	4.455257	2.112107
H	0.221521	5.317933	2.260023
H	0.277272	3.557696	2.479443
C	-2.035258	4.450076	0.930436

H	-1.967818	5.541130	0.903708
H	-3.026371	4.162367	0.572144
H	-1.933782	4.118895	1.964099
C	-1.307648	4.122626	-1.417677
H	-2.270960	3.664548	-1.652090
H	-1.384519	5.195595	-1.605817
H	-0.554426	3.702481	-2.088588

Py-OH

Energy = -690.704391

C	-0.677623	-3.695332	0.000000
C	0.649118	-3.296498	0.000000
C	0.987412	-1.942487	0.000000
C	-0.050362	-0.974028	0.000000
C	-1.405539	-1.392179	0.000000
C	-1.696415	-2.757376	0.000000
C	2.347267	-1.496867	0.000000
C	0.268332	0.410514	0.000000
C	1.626077	0.818537	0.000000
C	2.649600	-0.179279	0.000000
C	1.912960	2.182884	0.000000
H	2.949524	2.503998	0.000000
C	0.902113	3.124862	0.000000
C	-0.429778	2.730384	0.000000
C	-0.773840	1.371170	0.000000
C	-2.130782	0.923700	0.000000
C	-2.430352	-0.395106	0.000000

H	-3.464477	-0.724734	0.000000
H	-2.921761	1.663644	0.000000
H	3.131408	-2.247175	0.000000
H	-0.920832	-4.751957	0.000000
H	1.443423	-4.036085	0.000000
H	-2.734653	-3.073289	0.000000
H	3.683789	0.150858	0.000000
H	1.137160	4.184655	0.000000
O	-1.439608	3.629611	0.000000
H	-1.080757	4.525178	0.000000

Vibrational frequencies for the compounds Py-Bor and **Py-OH respectively.**

Py-Bor

mode	wave number	IR intensity	selection rules
1	20.8364	0.0426	YES
2	37.8737	1.3112	YES
3	73.8725	1.1625	YES
4	85.6997	0.3376	YES
5	109.9001	1.4551	YES
6	118.0709	0.3287	YES
7	178.1747	0.2805	YES
8	188.8987	0.3216	YES
9	209.4570	12.5506	YES
10	211.5325	2.0831	YES
11	225.9563	0.0237	YES
12	240.6951	0.2438	YES

13	254.5513	0.0636	YES
14	274.7565	0.3571	YES
15	289.6408	1.1758	YES
16	299.5923	0.2165	YES
17	317.6775	0.1719	YES
18	355.4576	1.6259	YES
19	369.9681	0.1247	YES
20	370.3727	0.6731	YES
21	391.6881	1.5437	YES
22	402.1421	1.3184	YES
23	415.0604	4.5256	YES
24	421.1695	0.1417	YES
25	451.7269	5.9659	YES
26	476.3024	0.3628	YES
27	478.4799	0.9646	YES
28	483.4987	0.5053	YES
29	507.2678	1.7786	YES
30	517.6902	8.8565	YES
31	525.0801	0.0443	YES
32	530.4260	1.5627	YES
33	531.4130	3.9858	YES
34	553.6502	7.7356	YES
35	577.4899	2.0612	YES
36	590.6715	6.0653	YES
37	599.2853	3.9848	YES
38	621.7591	0.7641	YES
39	628.7462	5.1814	YES

40	642.0383	33.5379	YES
41	693.1953	13.6483	YES
42	701.5506	49.5666	YES
43	704.0611	1.9253	YES
44	751.8021	3.5485	YES
45	767.3739	5.1764	YES
46	794.1034	10.8574	YES
47	806.5038	8.1599	YES
48	822.3119	129.0658	YES
49	830.1191	25.2580	YES
50	849.8709	102.7368	YES
51	859.6550	7.2335	YES
52	870.2893	39.0584	YES
53	889.7744	51.7268	YES
54	913.0446	0.3456	YES
55	936.2794	0.1781	YES
56	941.8711	2.2448	YES
57	973.3002	0.9945	YES
58	976.6976	1.2729	YES
59	977.5364	7.4360	YES
60	979.3972	18.8498	YES
61	980.0153	33.5608	YES
62	986.2651	0.1458	YES
63	992.3577	14.8259	YES
64	997.1618	1.4953	YES
65	1014.2093	1.3468	YES
66	1052.8722	38.1499	YES

67	1099.8756	73.0581	YES
68	1122.3233	10.3733	YES
69	1128.3329	18.1866	YES
70	1142.2687	177.1797	YES
71	1153.0840	126.1901	YES
72	1162.5015	354.6514	YES
73	1173.8500	8.5874	YES
74	1181.7883	17.9600	YES
75	1185.1140	61.2463	YES
76	1211.9206	4.9171	YES
77	1239.0152	4.0081	YES
78	1243.9606	37.7133	YES
79	1260.2372	11.1082	YES
80	1267.4068	16.3274	YES
81	1276.2136	7.3502	YES
82	1298.4975	543.1704	YES
83	1309.5640	83.0186	YES
84	1328.1574	358.7432	YES
85	1338.3022	169.7388	YES
86	1374.6766	425.1315	YES
87	1380.4990	8.0359	YES
88	1381.5051	32.6326	YES
89	1391.4114	20.3144	YES
90	1398.0261	38.7107	YES
91	1400.8924	212.9721	YES
92	1416.9282	33.0722	YES
93	1425.3601	22.9410	YES

94	1435.9513	0.5752	YES
95	1438.0252	7.3473	YES
96	1440.0010	0.0632	YES
97	1443.4374	4.7590	YES
98	1448.6917	2.6121	YES
99	1457.0287	8.0595	YES
100	1458.3829	24.8109	YES
101	1463.9038	12.6329	YES
102	1470.7312	14.4410	YES
103	1476.3711	1.2029	YES
104	1495.3441	4.1890	YES
105	1526.3253	2.7167	YES
106	1543.5498	125.4708	YES
107	1579.4616	25.8243	YES
108	1630.3044	29.0862	YES
109	1641.6387	71.8709	YES
110	1659.3362	26.1828	YES
111	1683.1439	17.1299	YES
112	3037.9366	10.1256	YES
113	3039.7808	34.9262	YES
114	3041.7698	22.5005	YES
115	3044.2496	15.3253	YES
116	3118.5773	8.1156	YES
117	3119.5735	10.6833	YES
118	3122.4021	5.5926	YES
119	3123.4898	90.5520	YES
120	3131.4741	32.7555	YES

121	3134.9581	37.9924	YES
122	3138.3369	24.3194	YES
123	3141.7341	28.9352	YES
124	3165.0858	4.2838	YES
125	3167.3435	6.8866	YES
126	3173.3065	14.1854	YES
127	3173.9141	19.9930	YES
128	3177.1738	12.2400	YES
129	3182.9634	31.8613	YES
130	3187.1422	35.9368	YES
131	3192.5847	41.2647	YES
132	3212.1784	19.3068	YES

Py-OH

mode	wave number	IR intensity	selection rules
1	90.1328	1.4949	YES
2	123.2747	1.8237	YES
3	196.9609	5.4788	YES
4	215.1033	21.9460	YES
5	256.9110	1.1556	YES
6	259.1260	11.7495	YES
7	311.1235	0.2911	YES
8	365.9026	170.7755	YES
9	392.1040	0.7685	YES
10	424.2960	0.0939	YES
11	424.4415	9.0311	YES
12	451.8645	7.8406	YES

13	456.5109	1.3258	YES
14	482.1597	0.0587	YES
15	491.4803	16.3912	YES
16	510.2121	2.4977	YES
17	530.5491	5.0277	YES
18	536.6336	0.0487	YES
19	557.4848	0.1148	YES
20	587.9198	0.6353	YES
21	613.0618	1.7755	YES
22	633.7615	0.0379	YES
23	641.8334	9.3085	YES
24	699.8587	4.0974	YES
25	716.9030	4.2896	YES
26	767.9893	6.8009	YES
27	777.4933	12.6673	YES
28	799.1732	0.0274	YES
29	811.2775	19.3676	YES
30	828.8891	242.9895	YES
31	830.1376	18.8911	YES
32	909.1317	0.1559	YES
33	916.2746	83.5933	YES
34	920.5976	1.4858	YES
35	975.9028	0.6252	YES
36	980.9021	0.1633	YES
37	990.9876	0.2150	YES
38	992.1600	22.0588	YES
39	1075.5907	32.6516	YES

40	1108.5347	81.7271	YES
41	1121.1138	34.4854	YES
42	1130.1143	24.5747	YES
43	1146.5859	9.7510	YES
44	1176.1176	34.7771	YES
45	1181.3328	49.7148	YES
46	1228.6355	74.1448	YES
47	1240.7948	30.5676	YES
48	1257.0589	11.5618	YES
49	1261.4704	3.7573	YES
50	1288.9737	441.9842	YES
51	1341.7180	40.3857	YES
52	1363.0823	117.2667	YES
53	1409.3657	1.5919	YES
54	1422.1445	32.7306	YES
55	1438.6847	11.4473	YES
56	1443.7657	39.7370	YES
57	1460.4729	50.2317	YES
58	1496.6964	8.0900	YES
59	1526.9144	56.0723	YES
60	1547.7054	275.0468	YES
61	1602.5084	25.3506	YES
62	1644.3510	67.9279	YES
63	1649.1011	14.0557	YES
64	1655.8704	67.8013	YES
65	1684.1320	65.3424	YES
66	3167.1864	6.2074	YES

67	3169.8045	4.3556	YES
68	3170.3817	16.9350	YES
69	3171.2728	10.8565	YES
70	3177.9499	23.2810	YES
71	3182.9325	24.6669	YES
72	3185.7855	31.7071	YES
73	3191.3639	45.4082	YES
74	3205.1553	15.0665	YES
75	3819.6717	345.1885	YES