

## Supporting Information

for

### A New Ratiometric and Colorimetric Chemosensor for Cyanide

#### Anion based on Coumarin-hemicyanine Hybrid

Zhenghao Yang,<sup>a</sup> Zhipeng Liu,<sup>\*a,b</sup> Yuncong Chen,<sup>b</sup> Xiaoqing Wang,<sup>c</sup> Weijiang He<sup>\*b</sup> and Yi Lu<sup>d</sup>

- State Key Laboratory of Coordination Chemistry, Coordination Chemistry Institute, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, P.R. China.
- Shandong Provincial Key Laboratory of Chemical Energy Storage and Novel Cell Technology, School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252000, P.R. China.
- School of Material Science and Engineering, Liaocheng University, Liaocheng 252000, P.R. China.
- Department of Chemistry, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA.

Email: chliuzp@163.com; hewej69@nju.edu.cn

#### 1. <sup>1</sup>H NMR and ESI-MS Spectra of Cou-BT.

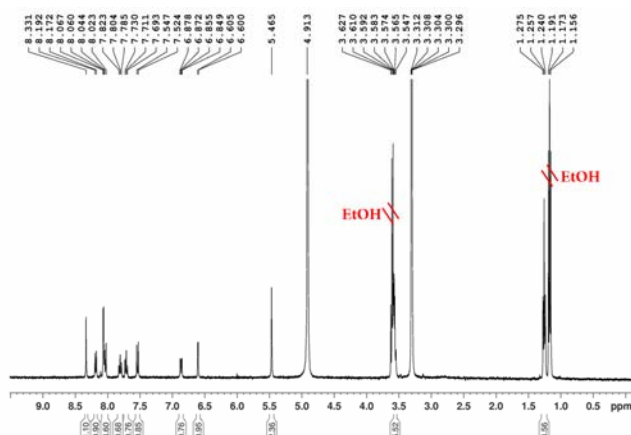


Figure S1. <sup>1</sup>H NMR spectrum of Cou-BT.

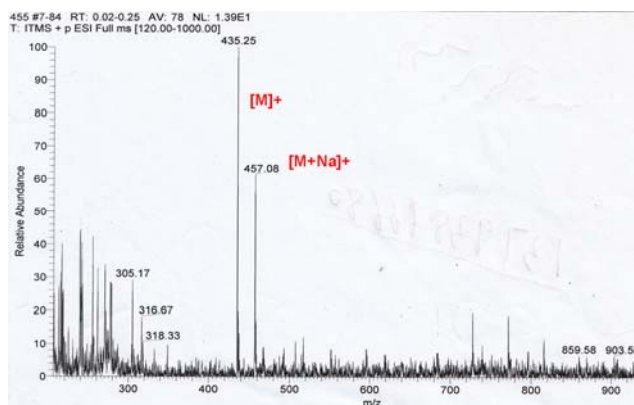


Figure S2. ESI-MS spectrum of Cou-BT.

## 2. Simulated UV-Vis absorption spectra for Cou-BT and Cou-BT-CN.

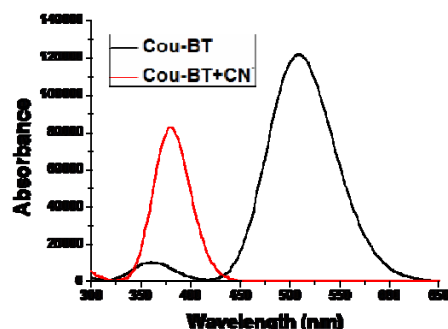


Figure S3. Simulated UV-Vis absorption spectra for Cou-BT and Cou-BT-CN.

## 3. Z-matrix and total energy of Cou-BT and Cou-BT-CN

### Cou-BT (TDDFT B3LYP 6-31G(d,p))

Symbolic Z-matrix:

Charge = 1 Multiplicity = 1

C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	5	B5	4	A4	3	D3	0
H	3	B6	2	A5	1	D4	0
H	1	B7	2	A6	3	D5	0
H	2	B8	1	A7	6	D6	0
C	3	B9	2	A8	1	D7	0
H	5	B10	4	A9	3	D8	0
C	4	B11	3	A10	2	D9	0
C	10	B12	3	A11	2	D10	0
C	6	B13	5	A12	4	D11	0
C	14	B14	6	A13	5	D12	0
H	14	B15	6	A14	5	D13	0
H	14	B16	6	A15	5	D14	0
H	15	B17	14	A16	6	D15	0
H	15	B18	14	A17	6	D16	0
H	15	B19	14	A18	6	D17	0
C	6	B20	5	A19	4	D18	0
C	21	B21	6	A20	5	D19	0
H	21	B22	6	A21	5	D20	0
H	21	B23	6	A22	5	D21	0
H	22	B24	21	A23	6	D22	0
H	22	B25	21	A24	6	D23	0

H	22	B26	21	A25	6	D24	0
N	6	B27	5	A26	4	D25	0
O	4	B28	3	A27	2	D26	0
O	12	B29	4	A28	3	D27	0
C	13	B30	10	A29	3	D28	0
C	31	B31	13	A30	10	D29	0
H	31	B32	13	A31	10	D30	0
H	32	B33	31	A32	13	D31	0
C	32	B34	31	A33	13	D32	0
C	35	B35	32	A34	31	D33	0
C	36	B36	35	A35	32	D34	0
C	36	B37	35	A36	32	D35	0
C	37	B38	36	A37	35	D36	0
C	38	B39	36	A38	35	D37	0
H	38	B40	36	A39	35	D38	0
C	39	B41	37	A40	36	D39	0
H	39	B42	37	A41	36	D40	0
H	40	B43	38	A42	36	D41	0
H	42	B44	39	A43	37	D42	0
S	35	B45	32	A44	31	D43	0
C	35	B46	32	A45	31	D44	0
H	47	B47	35	A46	32	D45	0
H	47	B48	35	A47	32	D46	0
C	47	B49	35	A48	32	D47	0
O	50	B50	47	A49	35	D48	0
O	50	B51	47	A50	35	D49	0
H	52	B52	50	A51	47	D50	0
N	35	B53	32	A52	31	D51	0

Variables:

B1	1.36992
B2	1.42309
B3	1.42184
B4	1.37787
B5	1.42446
B6	2.14712
B7	1.08125
B8	1.08701
B9	1.39843
B10	1.08107
B11	2.42939
B12	1.39714
B13	2.47025
B14	1.53408
B15	1.09307

B16	1.09464
B17	1.09594
B18	1.09446
B19	1.0948
B20	2.47603
B21	1.53395
B22	1.09442
B23	1.09295
B24	1.09602
B25	1.09496
B26	1.09441
B27	1.35942
B28	1.36512
B29	1.213
B30	1.42485
B31	1.37707
B32	1.09071
B33	1.08152
B34	1.41433
B35	2.33027
B36	1.40362
B37	1.39903
B38	1.39479
B39	1.39371
B40	1.08459
B41	1.39431
B42	1.08553
B43	1.08554
B44	1.08552
B45	1.74696
B46	2.47608
B47	1.09185
B48	1.0926
B49	1.53101
B50	1.20649
B51	1.34359
B52	0.97737
B53	1.35813
A1	121.62605
A2	116.70312
A3	122.79781
A4	120.17461
A5	98.67444
A6	118.50313

A7	119.5691
A8	125.05628
A9	117.61882
A10	91.76945
A11	122.31092
A12	90.68537
A13	107.85747
A14	131.8672
A15	87.28512
A16	109.47877
A17	111.29031
A18	111.90503
A19	151.87405
A20	107.74642
A21	87.88873
A22	131.72494
A23	109.47471
A24	111.89598
A25	111.34024
A26	121.3939
A27	120.07582
A28	144.53322
A29	120.01535
A30	127.32719
A31	114.13561
A32	117.64771
A33	123.7769
A34	157.26574
A35	80.14206
A36	159.46245
A37	121.51421
A38	118.11755
A39	121.88702
A40	117.96334
A41	121.04314
A42	119.06491
A43	119.488
A44	124.68707
A45	94.58935
A46	132.52262
A47	87.642
A48	107.2906
A49	124.87572
A50	109.60209

A51	108.75842
A52	124.14865
D1	0.26959
D2	-0.20767
D3	-0.6312
D4	-179.70897
D5	-179.37645
D6	-179.65731
D7	-179.80151
D8	179.11729
D9	179.78687
D10	179.96505
D11	-178.52808
D12	-71.89338
D13	148.2065
D14	39.02913
D15	149.46136
D16	-91.30195
D17	29.70523
D18	-179.01391
D19	-107.70842
D20	141.15847
D21	31.62079
D22	-149.80759
D23	-30.00706
D24	90.95167
D25	-178.12401
D26	179.51142
D27	-179.57546
D28	-179.47782
D29	179.26666
D30	-0.48284
D31	-0.62807
D32	-179.45104
D33	179.1778
D34	-177.59201
D35	-0.06581
D36	179.60716
D37	-177.69265
D38	1.55949
D39	-0.26937
D40	179.96228
D41	179.82675
D42	-179.85867

D43	2.12142
D44	-178.34724
D45	142.93736
D46	32.9457
D47	-76.762
D48	-23.54632
D49	156.16694
D50	-178.34298
D51	-177.85293

SCF Done: E(RB+HF-LYP) = -1736.8613626 a.u.

Number of Imaginary frequencies: n.a.

### **Cou-BT-CN<sup>-</sup> (TDDFT B3LYP 6-31G(d,p))**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C

C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	5	B5	4	A4	3	D3	0
H	3	B6	2	A5	1	D4	0
H	1	B7	2	A6	3	D5	0
H	2	B8	1	A7	6	D6	0
C	3	B9	2	A8	1	D7	0
H	5	B10	4	A9	3	D8	0
C	4	B11	3	A10	2	D9	0
C	10	B12	3	A11	2	D10	0
C	6	B13	5	A12	4	D11	0
C	14	B14	6	A13	5	D12	0
H	14	B15	6	A14	5	D13	0
H	14	B16	6	A15	5	D14	0
H	15	B17	14	A16	6	D15	0
H	15	B18	14	A17	6	D16	0
H	15	B19	14	A18	6	D17	0
C	6	B20	5	A19	4	D18	0
C	21	B21	6	A20	5	D19	0
H	21	B22	6	A21	5	D20	0
H	21	B23	6	A22	5	D21	0
H	22	B24	21	A23	6	D22	0
H	22	B25	21	A24	6	D23	0
H	22	B26	21	A25	6	D24	0
N	6	B27	5	A26	4	D25	0
O	4	B28	3	A27	2	D26	0

O	12	B29	4	A28	3	D27	0
C	13	B30	10	A29	3	D28	0
C	31	B31	13	A30	10	D29	0
H	31	B32	13	A31	10	D30	0
H	32	B33	31	A32	13	D31	0
C	32	B34	31	A33	13	D32	0
C	35	B35	32	A34	31	D33	0
C	35	B36	32	A35	31	D34	0
C	36	B37	35	A36	32	D35	0
C	37	B38	35	A37	32	D36	0
H	37	B39	35	A38	32	D37	0
C	39	B40	37	A39	35	D38	0
H	38	B41	36	A40	35	D39	0
H	39	B42	37	A41	35	D40	0
H	41	B43	39	A42	37	D41	0
S	36	B44	35	A43	32	D42	0
C	35	B45	32	A44	31	D43	0
H	46	B46	35	A45	32	D44	0
H	46	B47	35	A46	32	D45	0
C	46	B48	35	A47	32	D46	0
O	49	B49	46	A48	35	D47	0
O	49	B50	46	A49	35	D48	0
H	51	B51	49	A50	46	D49	0
N	35	B52	32	A51	31	D50	0
C	53	B53	35	A52	32	D51	0
N	54	B54	53	A53	35	D52	0
C	53	B55	35	A54	32	D53	0

Variables:

B1	1.37991
B2	1.4122
B3	1.40968
B4	1.38737
B5	1.41558
B6	2.16331
B7	1.08203
B8	1.08758
B9	1.42127
B10	1.08153
B11	2.43498
B12	1.37528
B13	2.4756
B14	1.53582
B15	1.09463
B16	1.09612



B17	1.0969
B18	1.09524
B19	1.09475
B20	2.48013
B21	1.53581
B22	1.09596
B23	1.09472
B24	1.09706
B25	1.09497
B26	1.09512
B27	1.37834
B28	1.36494
B29	1.21215
B30	1.45875
B31	1.34778
B32	1.09015
B33	1.08451
B34	3.65733
B35	1.4066
B36	1.39524
B37	1.38794
B38	1.40244
B39	1.08547
B40	1.39459
B41	1.08646
B42	1.08657
B43	1.0862
B44	1.7797
B45	2.47835
B46	1.10057
B47	1.09521
B48	1.52678
B49	1.20636
B50	1.35941
B51	0.97589
B52	1.4029
B53	2.42909
B54	1.16247
B55	1.47112
A1	121.69603
A2	116.72654
A3	122.77043
A4	120.2437
A5	99.10701

A6	118.33146
A7	119.36686
A8	125.39035
A9	117.33553
A10	91.70043
A11	122.5805
A12	90.81654
A13	107.81445
A14	132.63898
A15	87.29691
A16	109.84292
A17	111.21361
A18	111.64371
A19	151.65738
A20	108.02701
A21	87.57537
A22	132.3686
A23	109.91801
A24	111.57702
A25	111.21047
A26	121.34401
A27	120.169
A28	144.25989
A29	119.78491
A30	128.36392
A31	113.35376
A32	122.00441
A33	147.76277
A34	88.05165
A35	151.95375
A36	121.3856
A37	119.0917
A38	121.05846
A39	120.99209
A40	120.50225
A41	119.02729
A42	120.31858
A43	111.28091
A44	55.81597
A45	90.25434
A46	135.9809
A47	105.82633
A48	127.01229
A49	109.61362

A50	107.2348
A51	25.87237
A52	107.02792
A53	143.50548
A54	113.45143
D1	0.17952
D2	-0.10348
D3	-0.6735
D4	179.97869
D5	-179.28899
D6	-179.73521
D7	179.85583
D8	179.16076
D9	179.71687
D10	-179.9742
D11	-178.75172
D12	-71.48117
D13	148.12337
D14	38.88003
D15	148.04519
D16	-92.43798
D17	28.21025
D18	-178.69035
D19	-108.29749
D20	141.21704
D21	31.95845
D22	-148.35514
D23	-28.38722
D24	92.09178
D25	-178.05863
D26	179.55519
D27	-179.63213
D28	-179.68696
D29	177.6916
D30	-1.9116
D31	-0.19683
D32	164.98044
D33	97.87643
D34	-91.15949
D35	174.92041
D36	-169.1568
D37	9.90734
D38	-0.29297
D39	179.60187

D40	179.86851
D41	-179.71585
D42	-3.5282
D43	-73.70257
D44	139.99898
D45	25.81351
D46	-110.37766
D47	36.81034
D48	-143.70741
D49	-178.02165
D50	-75.08313
D51	65.13051
D52	75.92974
D53	28.23357

SCF Done: E(RB+HF-LYP) = -1829.8792918 a.u.

Number of Imaginary frequencies: n.a.