

Supporting Information

Introducing 3D conjugated acceptors with intense red absorption: homoleptic metal (II) complexes of di(phenylacetylene) azadipyrromethene

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NMR spectra for WS1 series

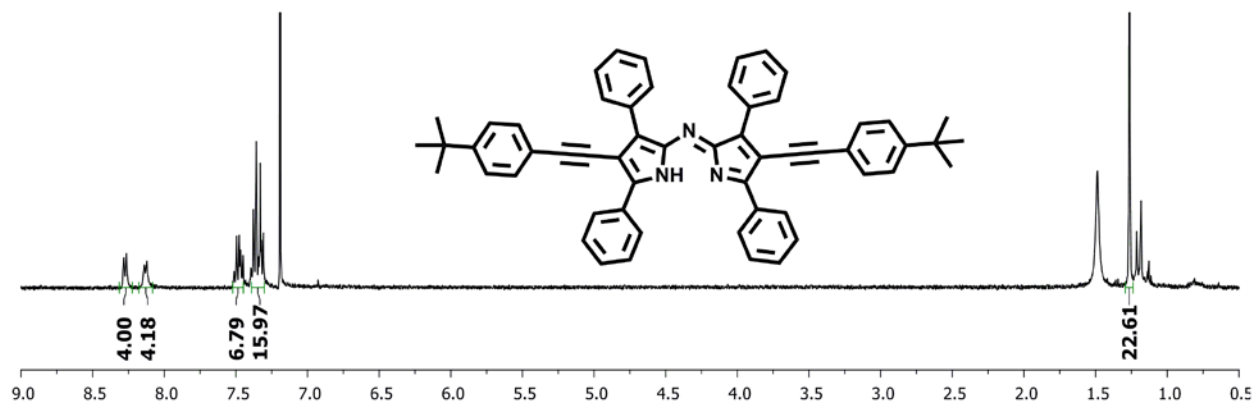


Figure S1: 400 MHz ¹H NMR of WS1.

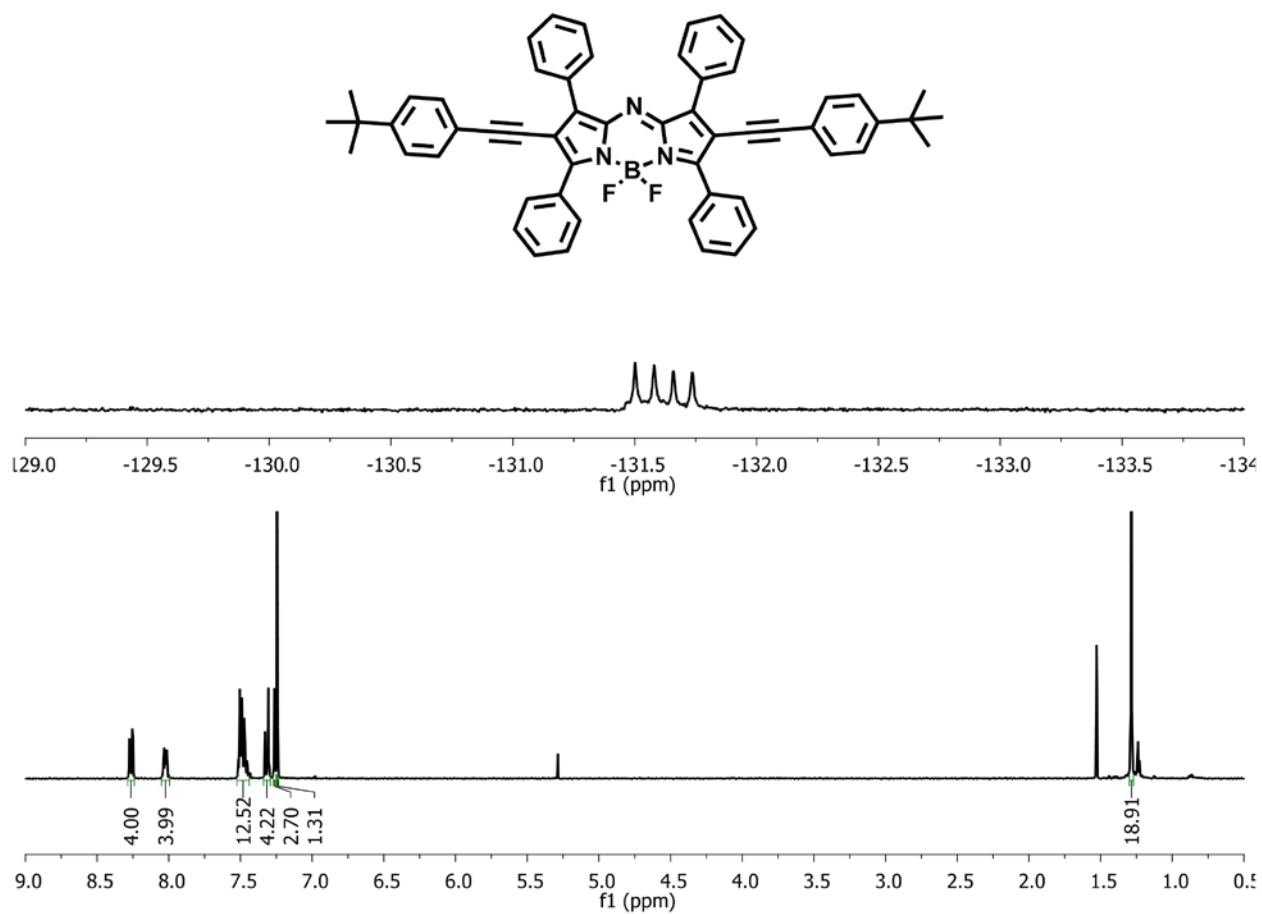


Figure S2: 400 MHz ¹H NMR (bottom) and ¹⁹F NMR (top) of WS1BF₂.

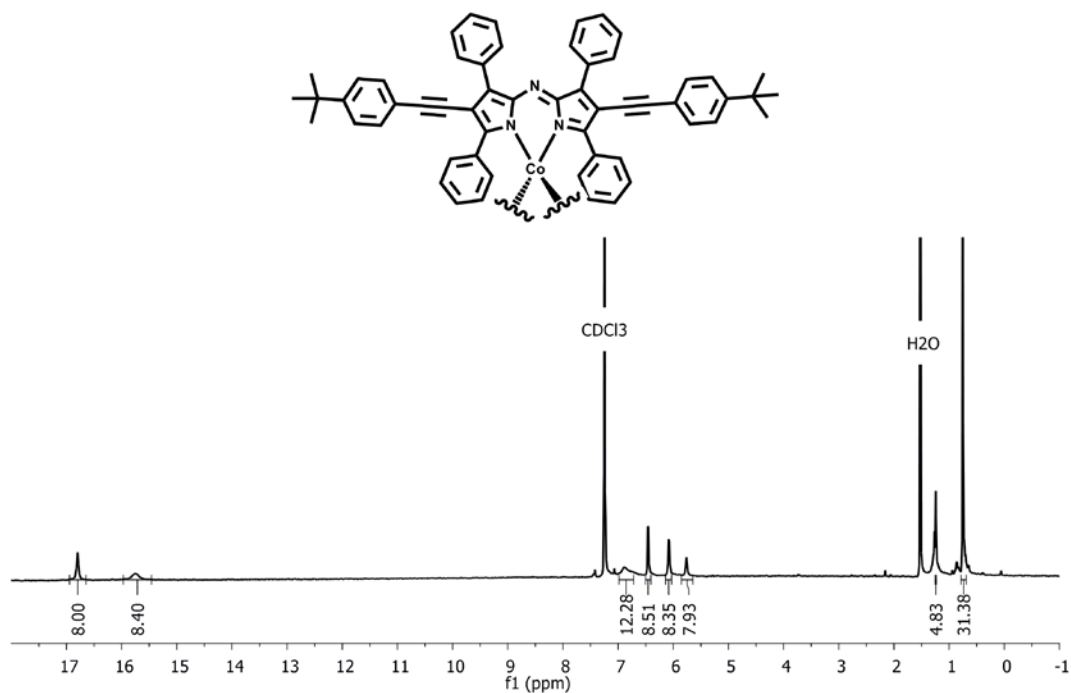


Figure S3: 400 MHz 1H NMR of $WS_{12}Co$

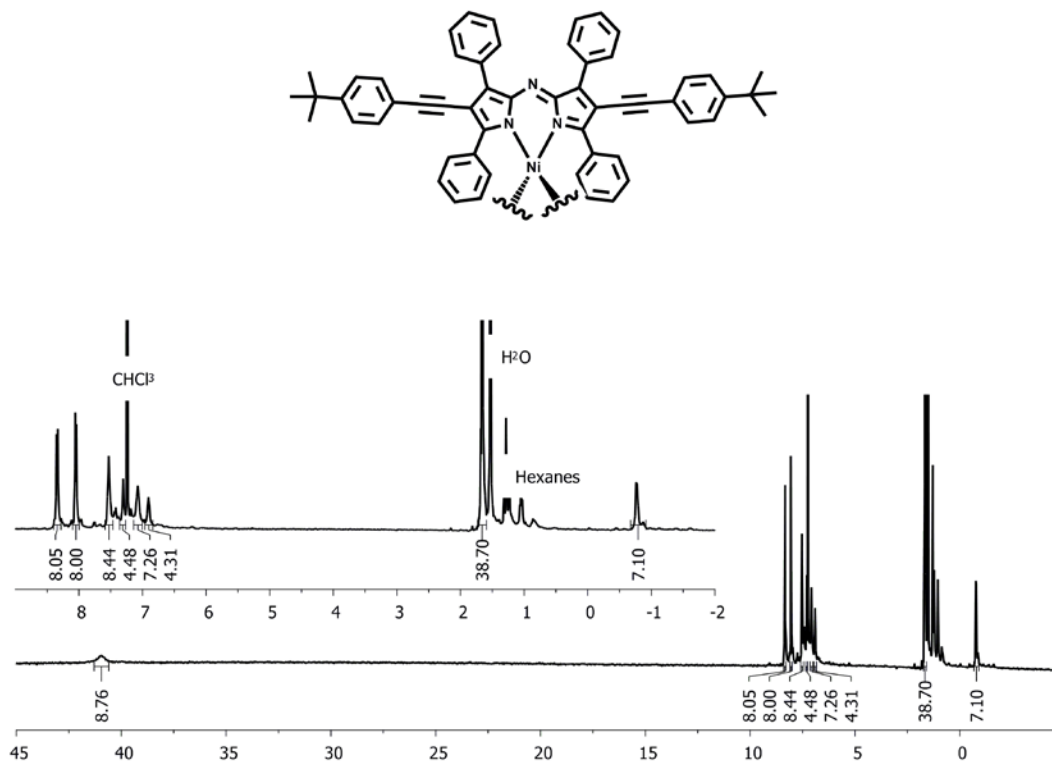


Figure S4: 400 MHz 1H NMR of $WS_{12}Ni$. Inset shows an expansion between -2 to 9 ppm.

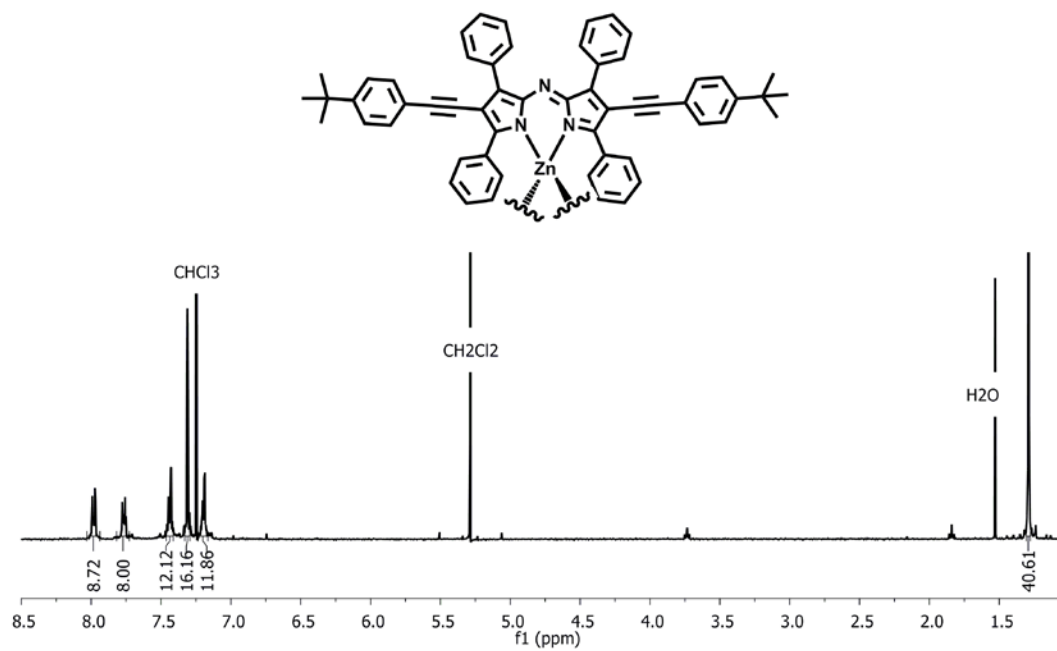


Figure S5: 400 MHz ¹H NMR of WS₁₂Zn.

MALDI-TOF-MS spectra for WS1 series

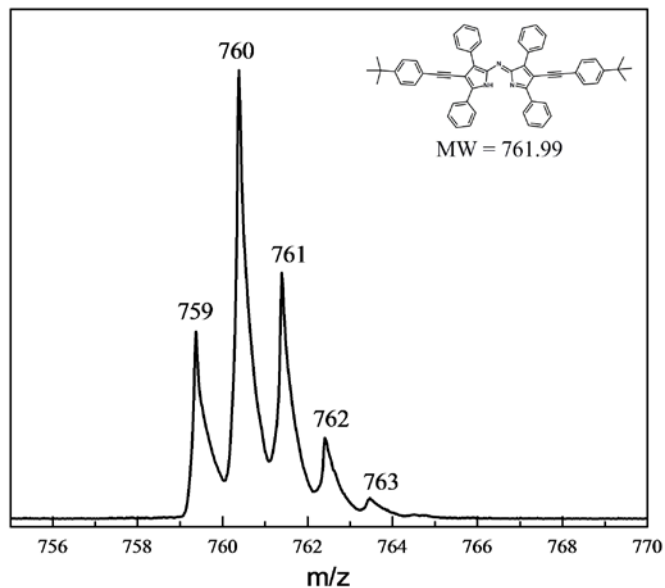


Figure S6: MALDI-TOF Mass Spectrum of WS1 (Isotope pattern of the molecular ion in reflective negative mode).

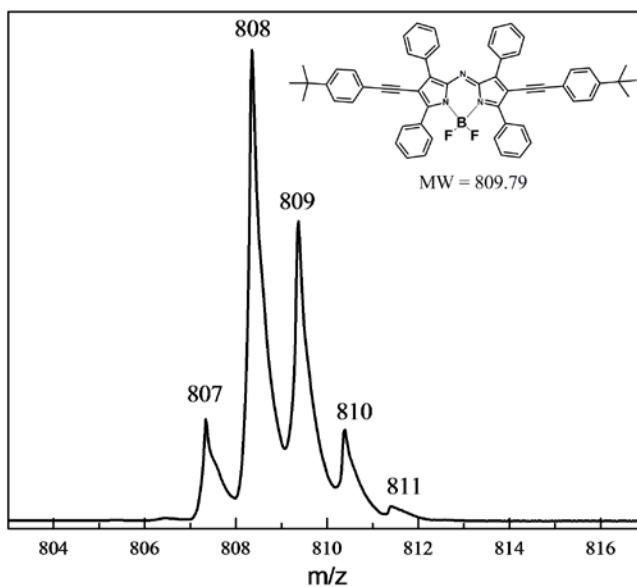


Figure S7: MALDI-TOF Mass Spectrum of WS1BF₂ (Isotope pattern of the molecular ion in reflective negative mode).

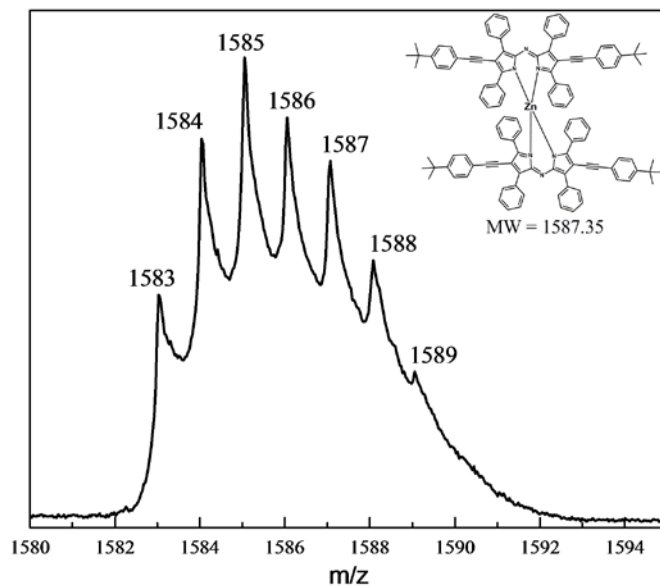


Figure S8: MALDI-TOF Mass Spectrum of WS₁₂Zn (Isotope pattern of the molecular ion in reflective negative mode).

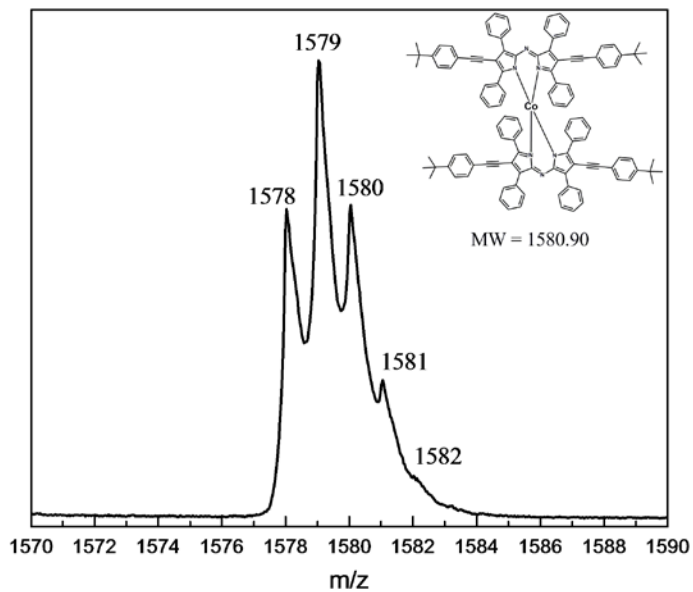


Figure S9: MALDI-TOF Mass Spectrum of WS₁₂Co (Isotope pattern of the molecular ion in reflective negative mode).

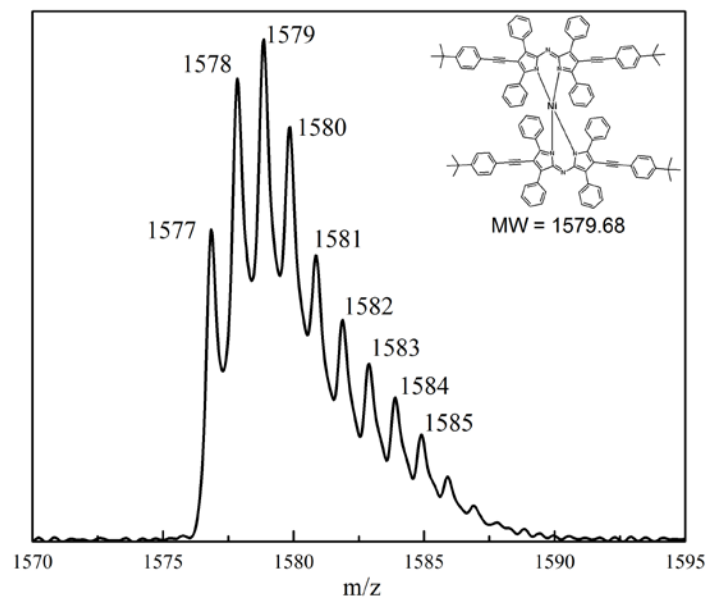


Figure S10: MALDI-TOF Mass Spectrum of WS₁₂Ni (Isotope pattern of the molecular ion in reflective negative mode).

Thermal gravimetric graphs for ADP and WS1 series

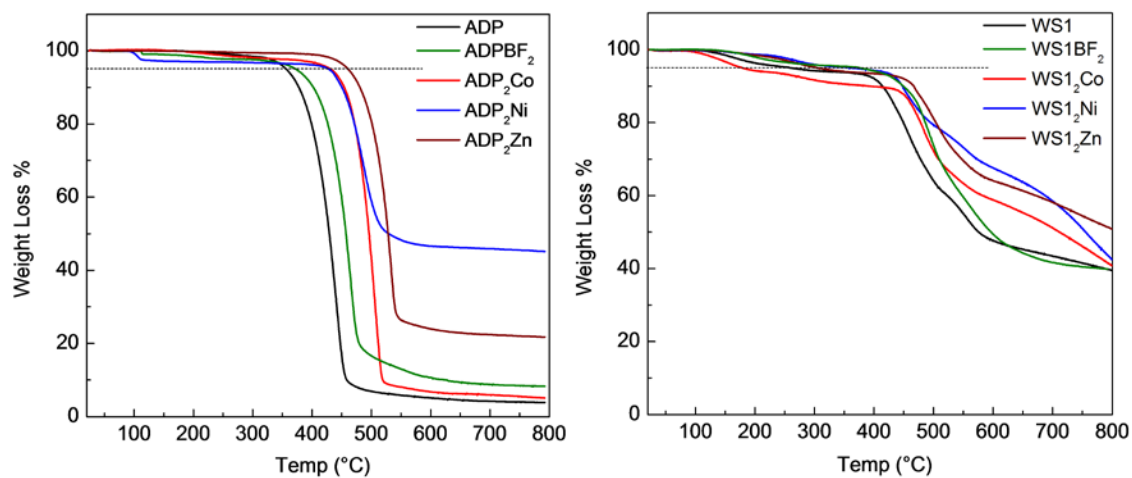


Figure S11: TGA graphs of ADP and WS1 series

Table S1: Decomposition temperature (°C) at 5% weight loss

	ADP	WS1
H	356	280
BF ₂	372	375
Co	431	240
Ni	428	360
Zn	461	304

Optical properties

Table S2: Optical properties

Compound	$\lambda_{\text{max near-UV, nm}}$ ($\epsilon, \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$)	$\lambda_{\text{max red, nm}}$ ($\epsilon, \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$)	$\lambda_{\text{max red-shoulder, nm}}$ ($\epsilon, \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$)	$\lambda_{\text{onsets, nm}}$	$E_{\text{gap, eV}}$
ADP	302 (38)	596 (42)		645	1.92
WS1	302 (46)	625 (47)		715	1.73
ADPBF ₂	310 (20)	649 (50)		688	1.80
WS1BF ₂	307 (32)	741 (48)		798	1.55
ADP ₂ Co	304 (56)	599 (61)	634 (37)	730	1.70
WS1 ₂ Co	315 (80)	670 (73)	703 (73)	793	1.56
ADP ₂ Ni	304 (52)	603 (50)	650 (45)	734	1.69
WS1 ₂ Ni	302 (80)	683 (67)	710 (68)	805	1.54
ADP ₂ Zn	302 (57)	591 (78)	645 (51)	713	1.74
WS1 ₂ Zn	300 (82)	650 (91)	683 (94)	764	1.62

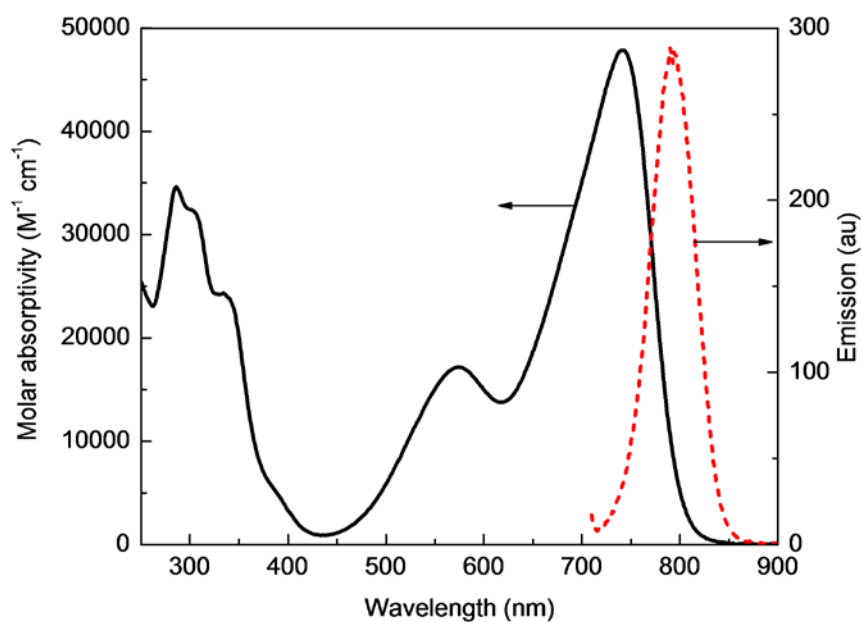


Figure S12: WS1BF₂ absorbance and emission in CHCl₃.

Cyclic voltammetry plots of ADP series

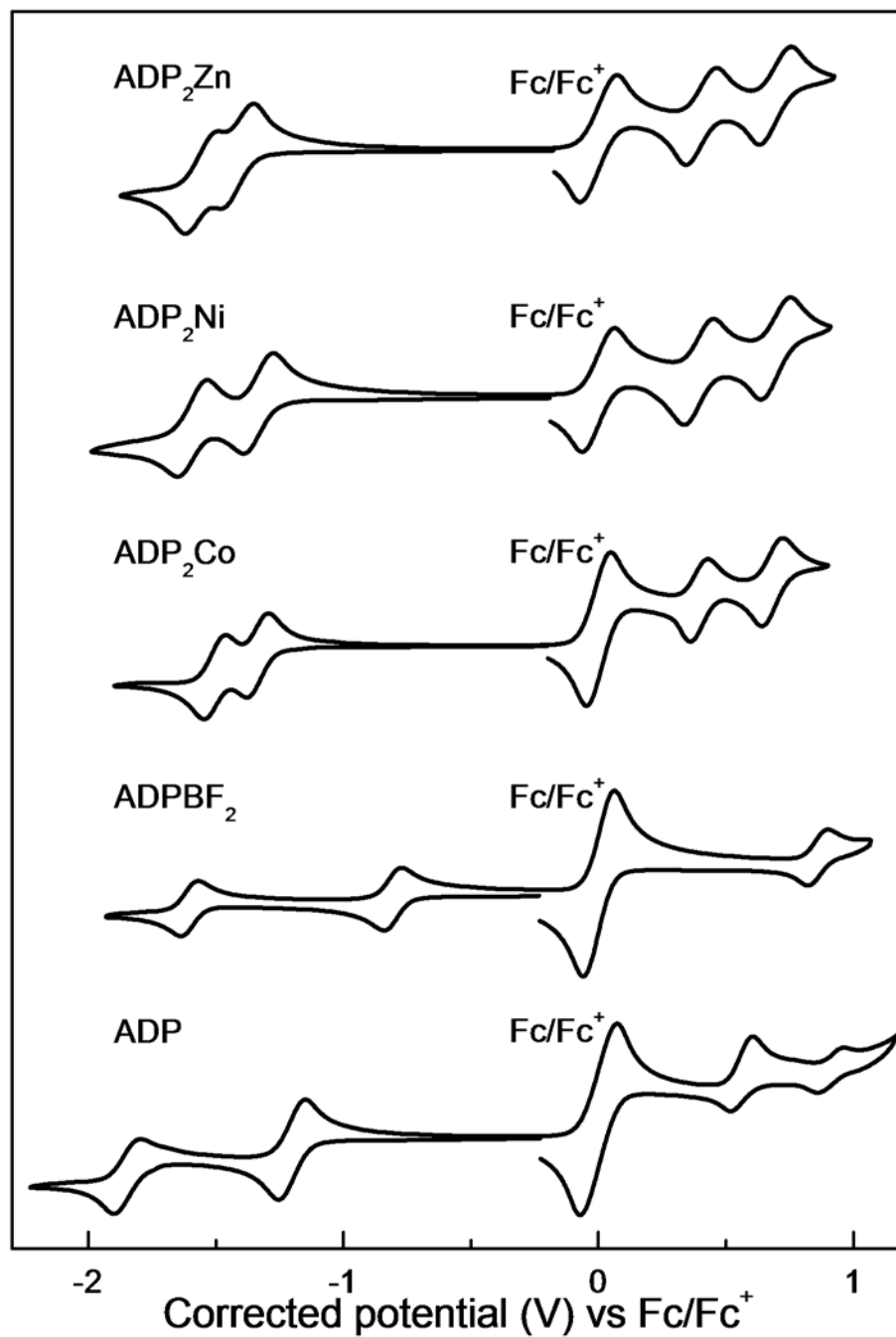


Figure S13: Cyclic voltammetry plots of ADP series measured in DCM/TBAPF (0.1 M) with Fc/Fc⁺ as internal standard, scan rate 100mV/s. Potentials are corrected to Fc/Fc⁺.

P3HT Fluorescence quenching in solution

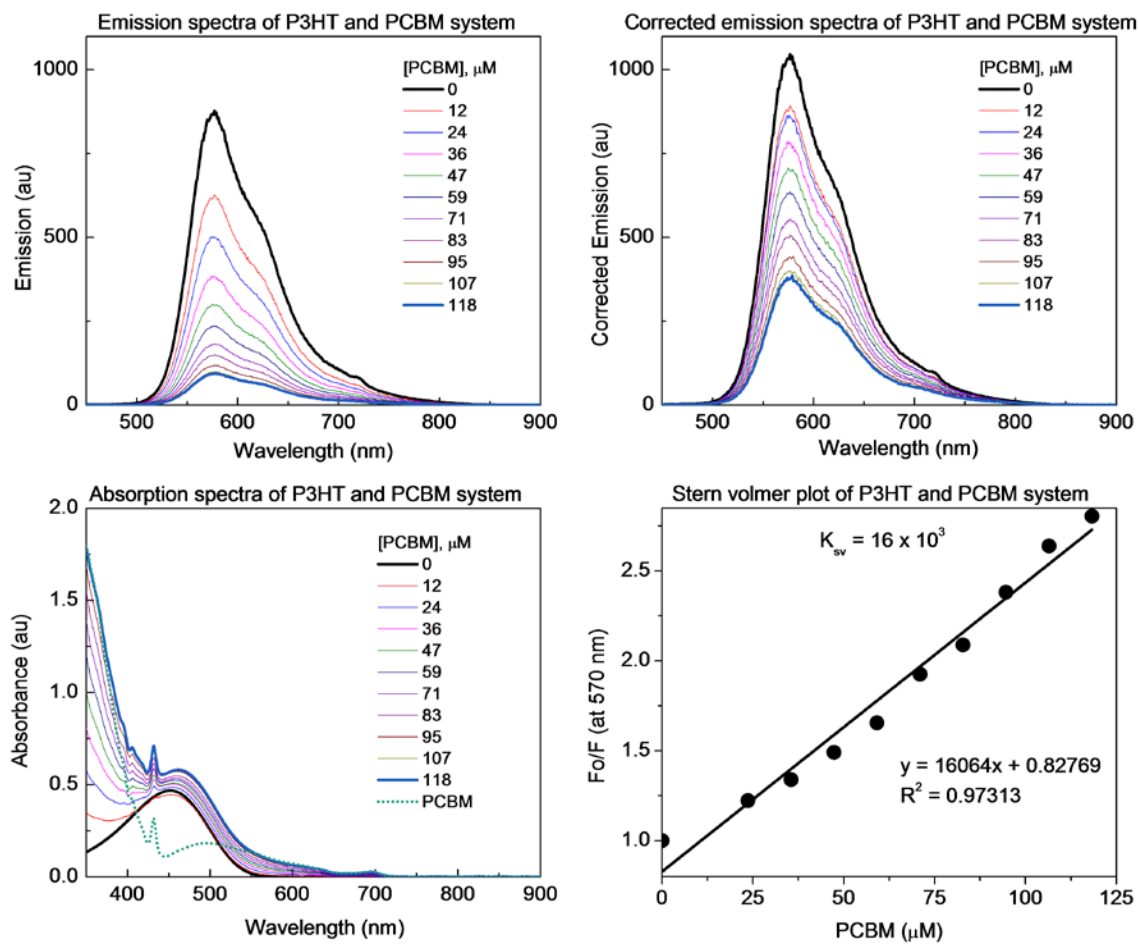


Figure S14: P3HT fluorescence quenching with PCBM.

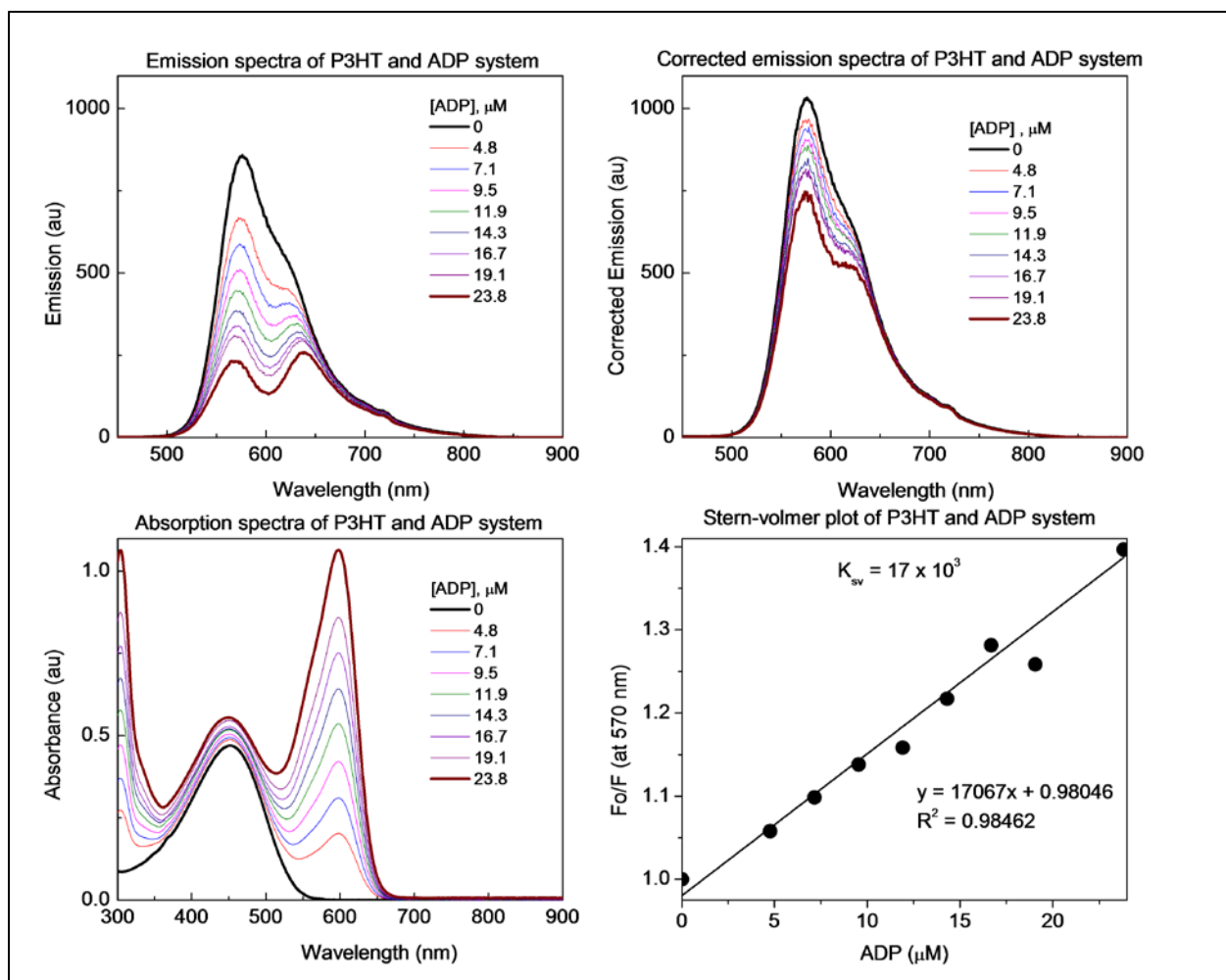


Figure S15: P3HT fluorescence quenching with ADP.

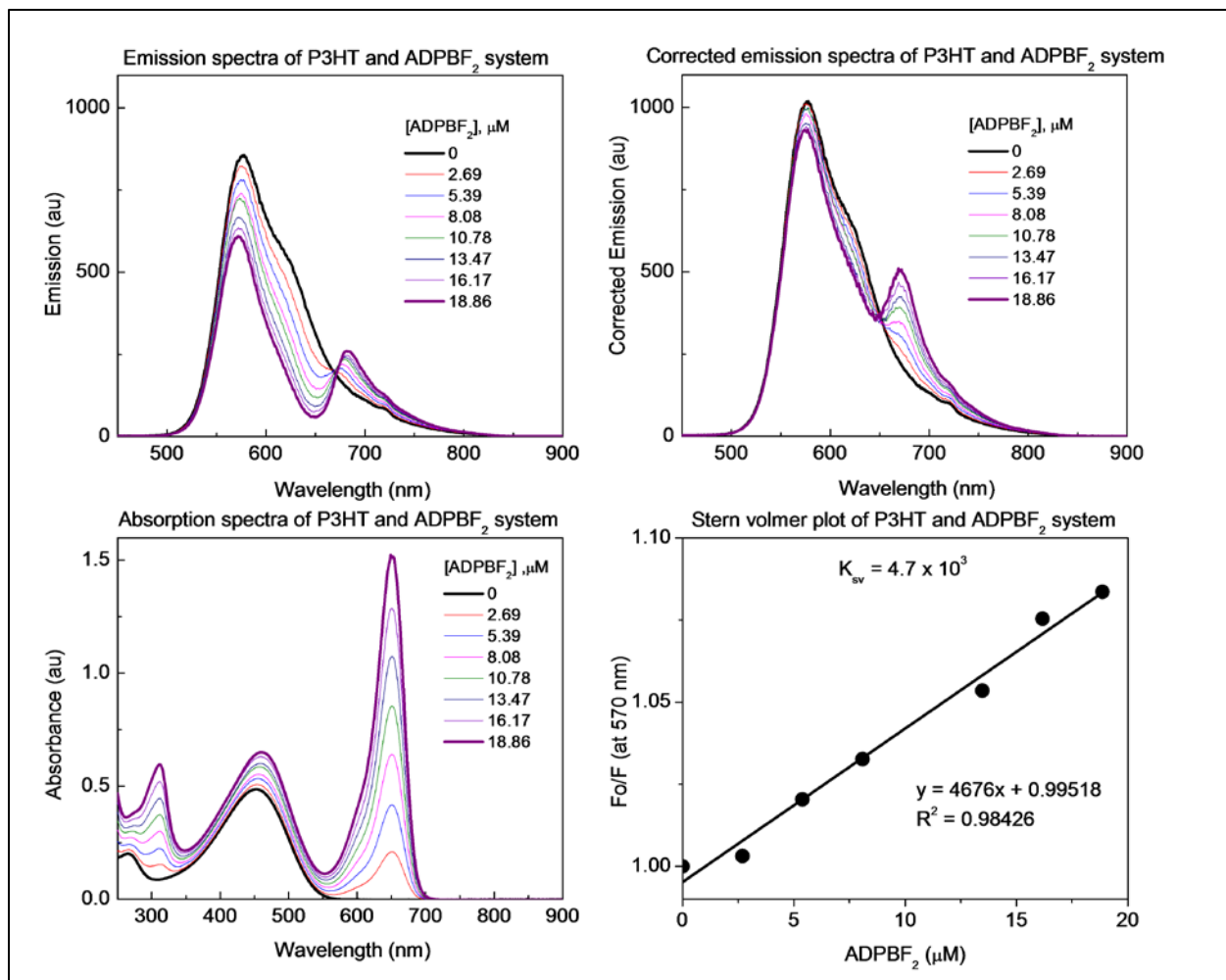


Figure S16: P3HT fluorescence quenching with ADPBF₂

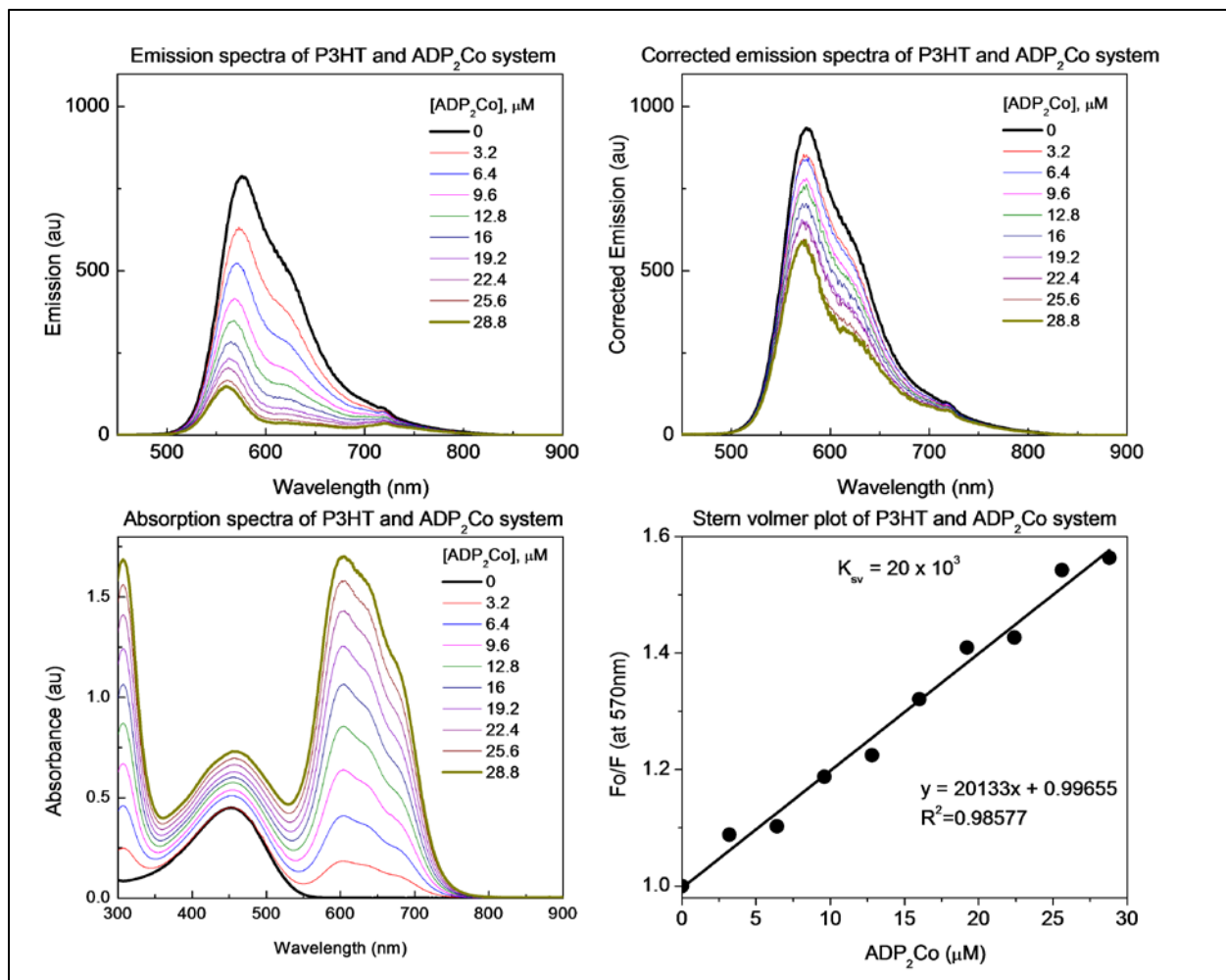


Figure S17: P3HT fluorescence quenching with ADP₂Co

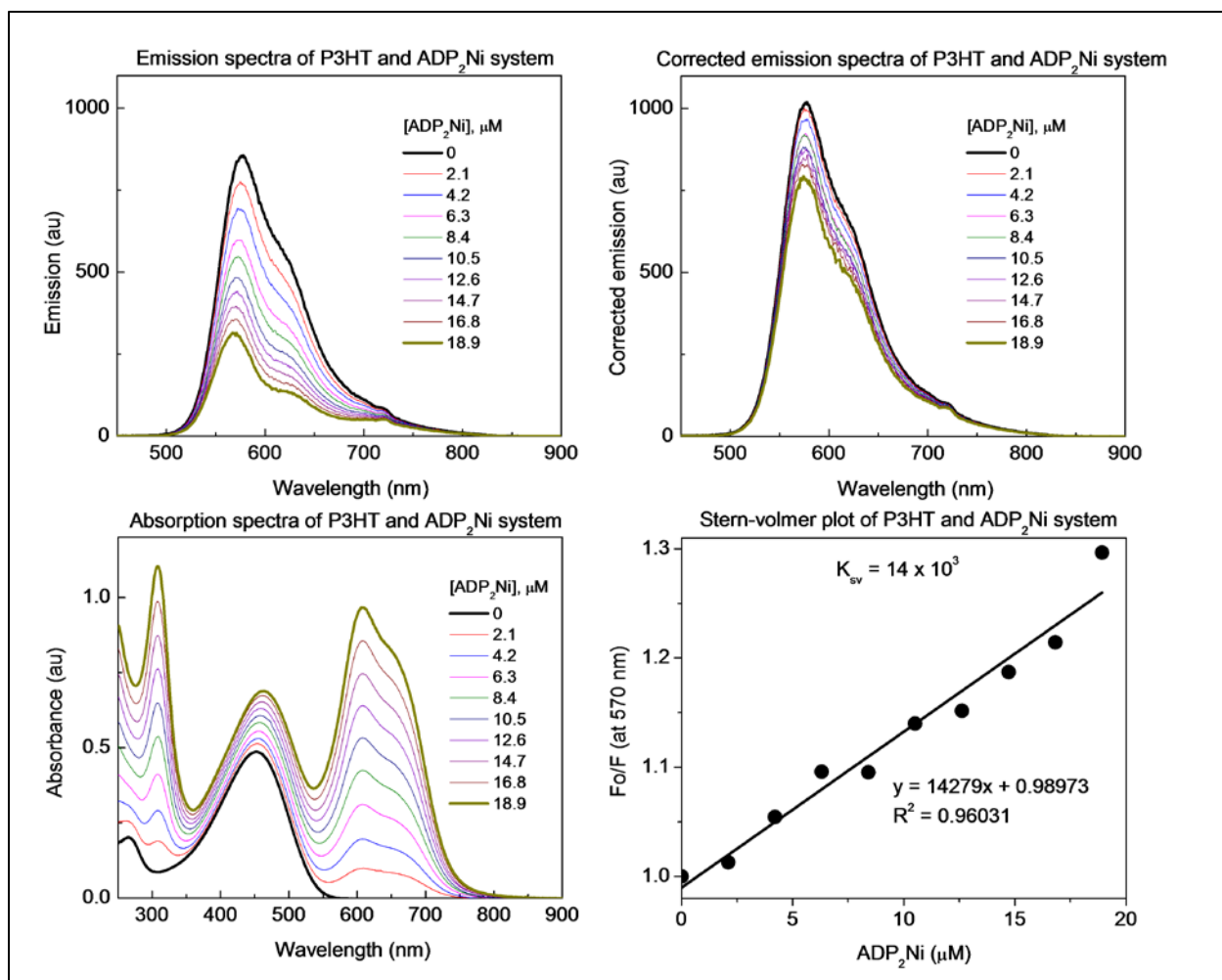


Figure S18: P3HT fluorescence quenching with ADP_2Ni

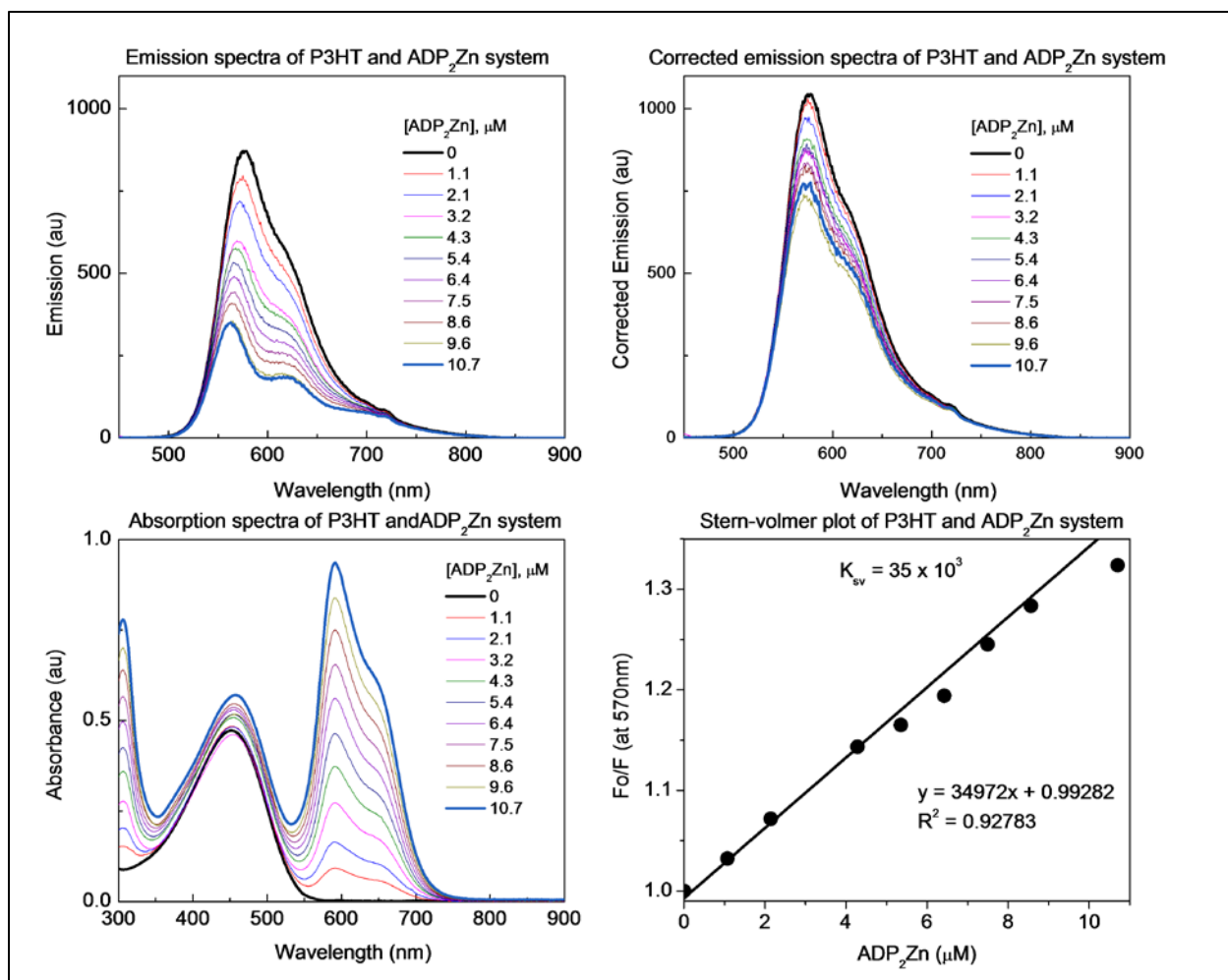


Figure S19: P3HT fluorescence quenching with ADP₂Zn.

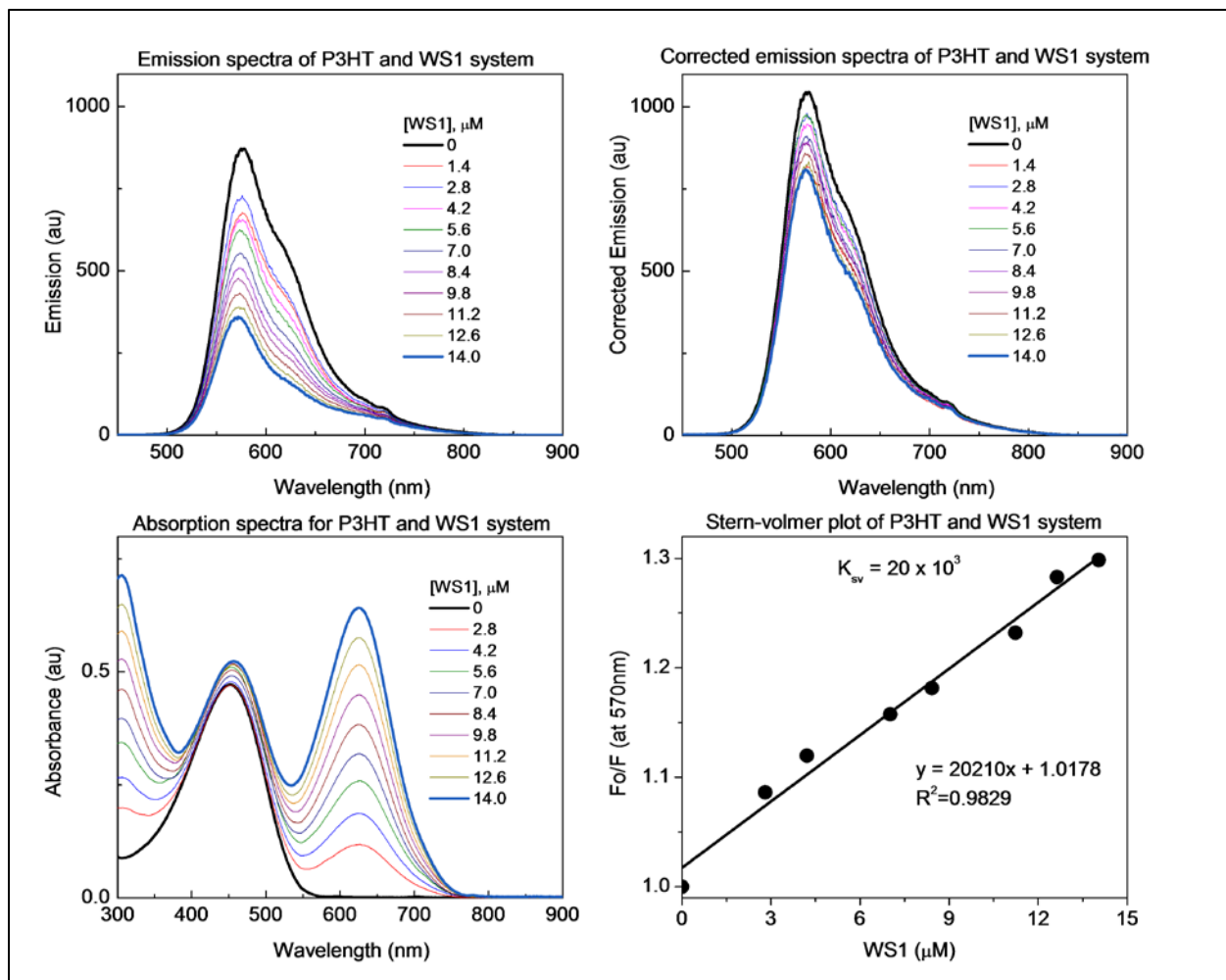


Figure S20: P3HT fluorescence quenching with WS1.

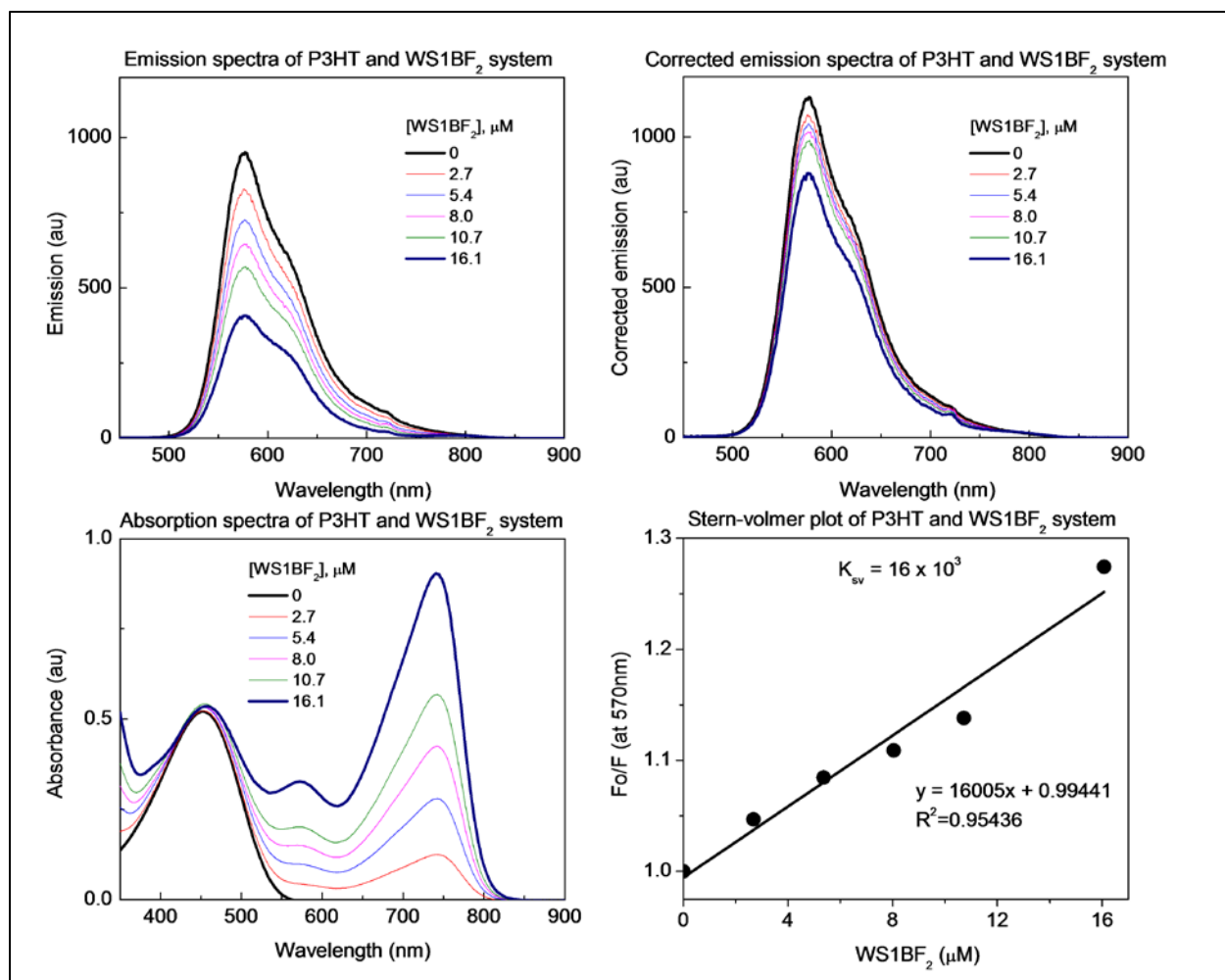


Figure S21: P3HT fluorescence quenching with WS1BF₂.

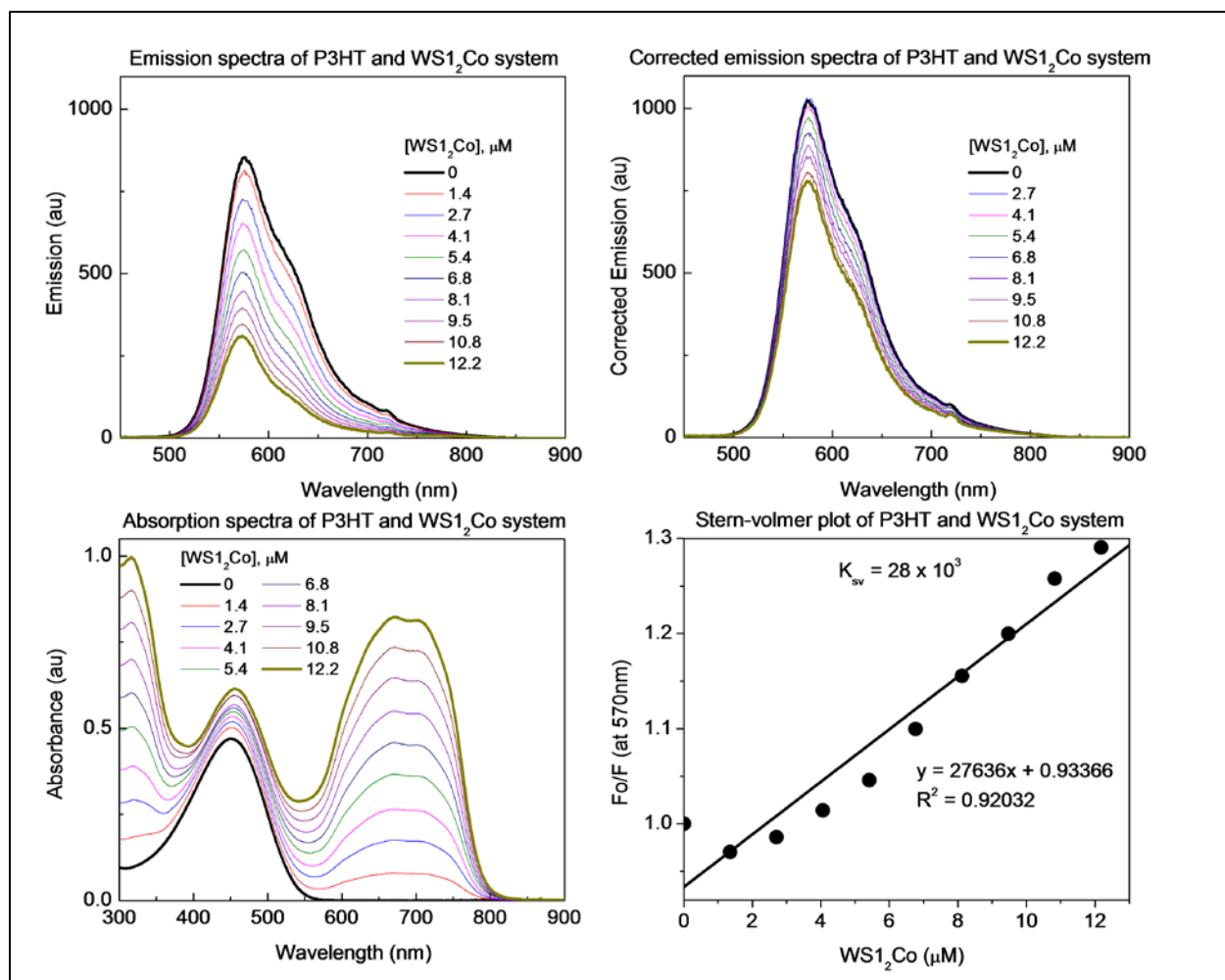


Figure S22: P3HT fluorescence quenching with WS₁₂Co.

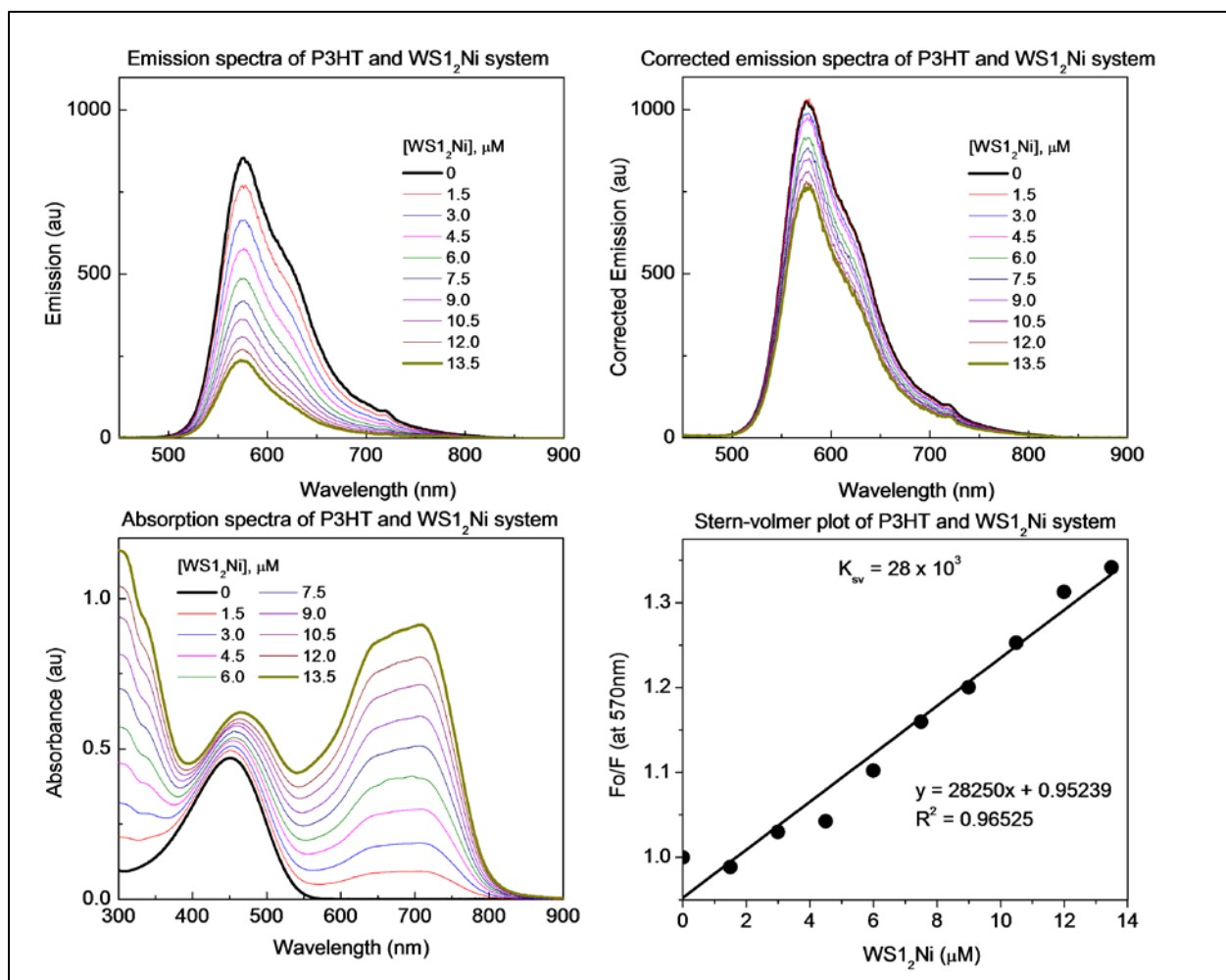


Figure S23: P3HT fluorescence quenching with WS₁₂Ni.

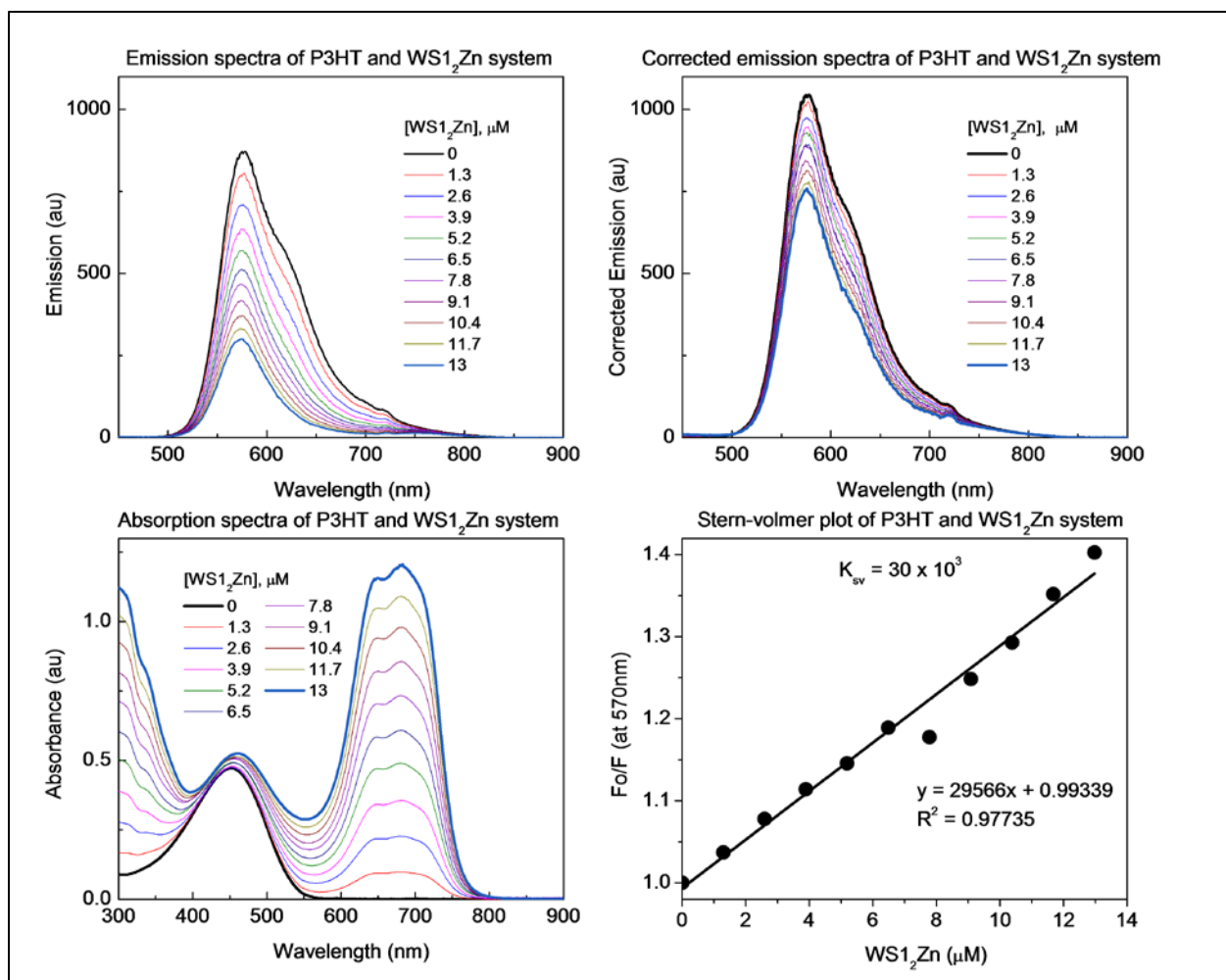


Figure S24: P3HT fluorescence quenching with WS₁₂Zn.

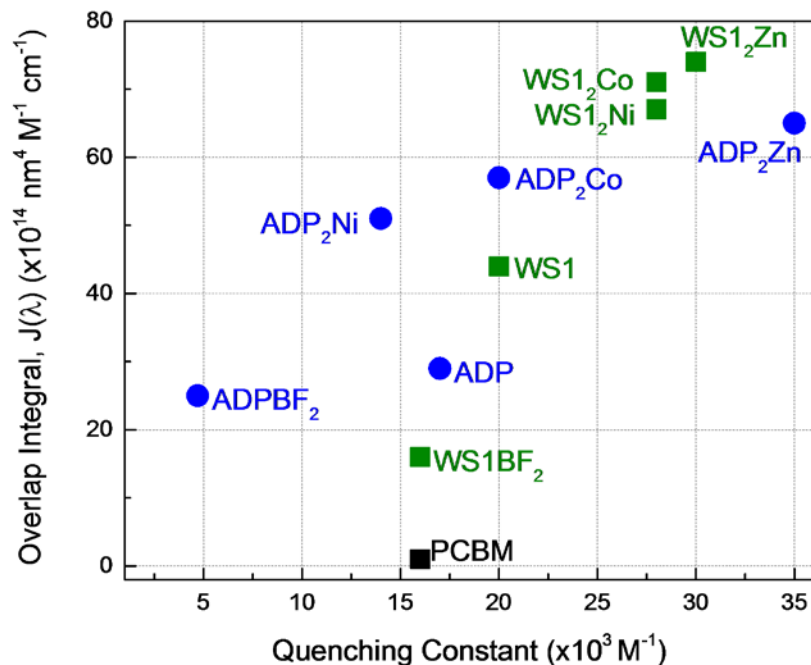


Figure S25: Plot of overlap integral versus Stern-Volmer (or quenching) constant for all compounds studied.

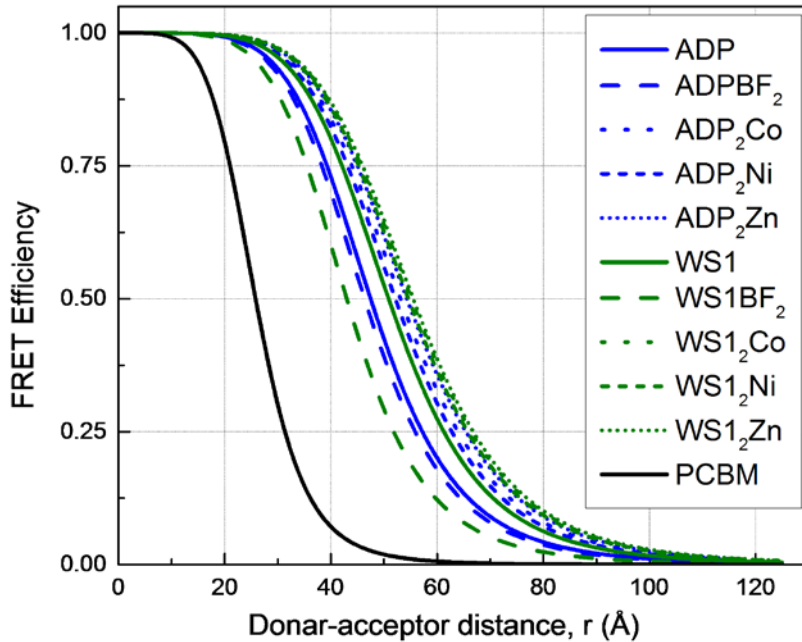


Figure S26: FRET efficiency as a function of donor-acceptor distance for PCBM and all aza-DIPY derivatives studied.

DFT Calculation

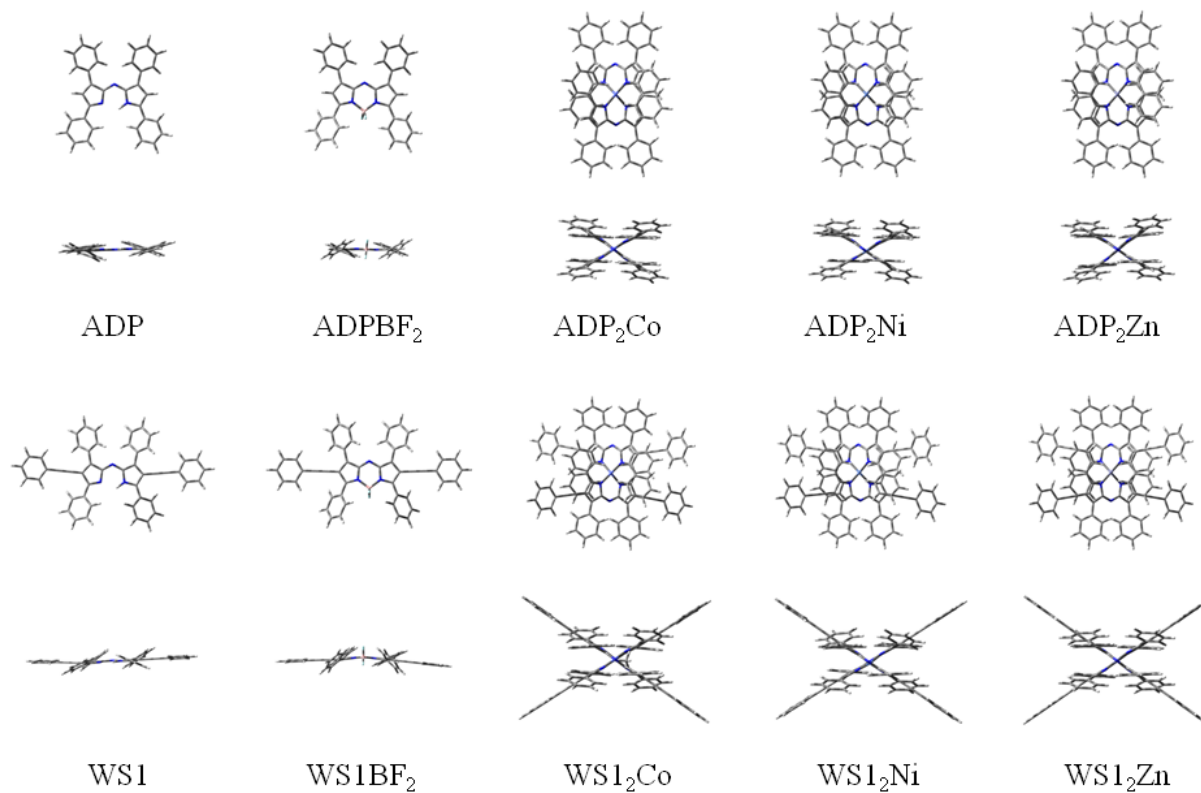


Figure S27: Optimized molecular structures of aza-DIPY molecules.

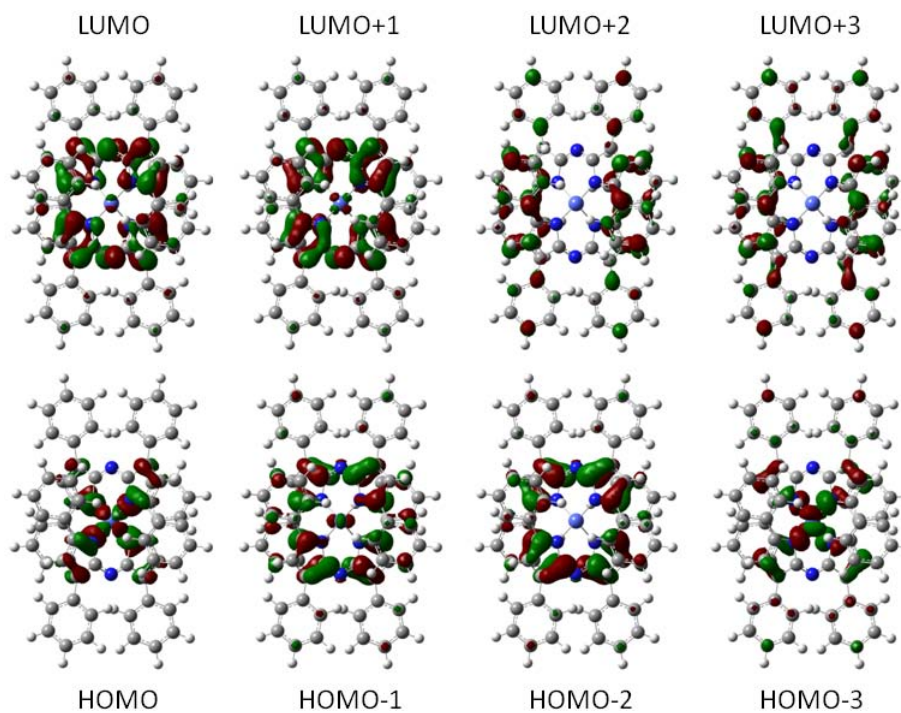


Figure S28: Calculated molecular orbital for ADP₂Co.

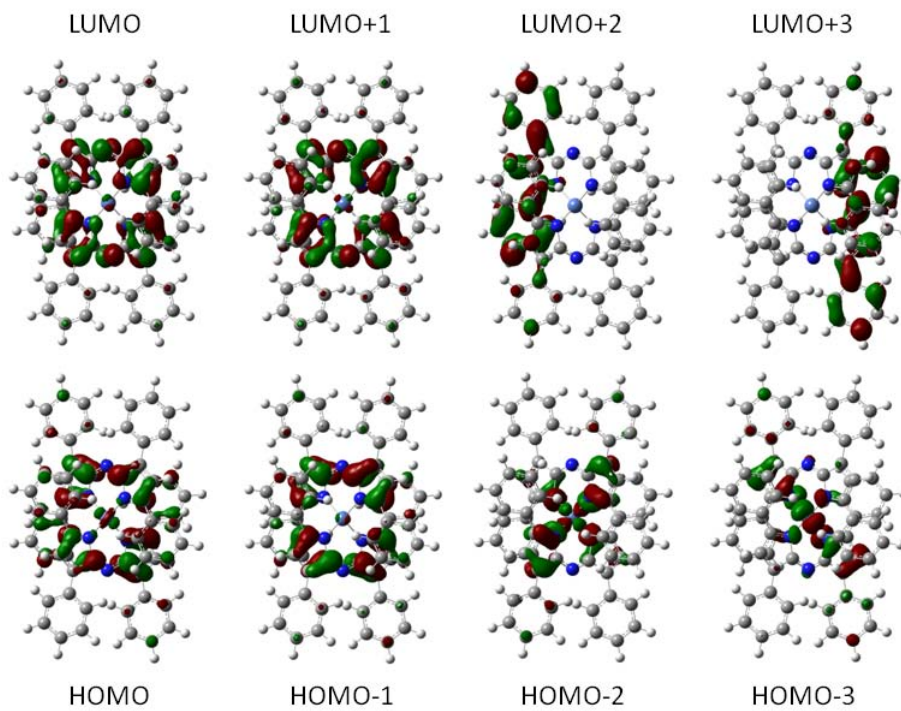


Figure S29: Calculated molecular orbital for ADP₂Ni.

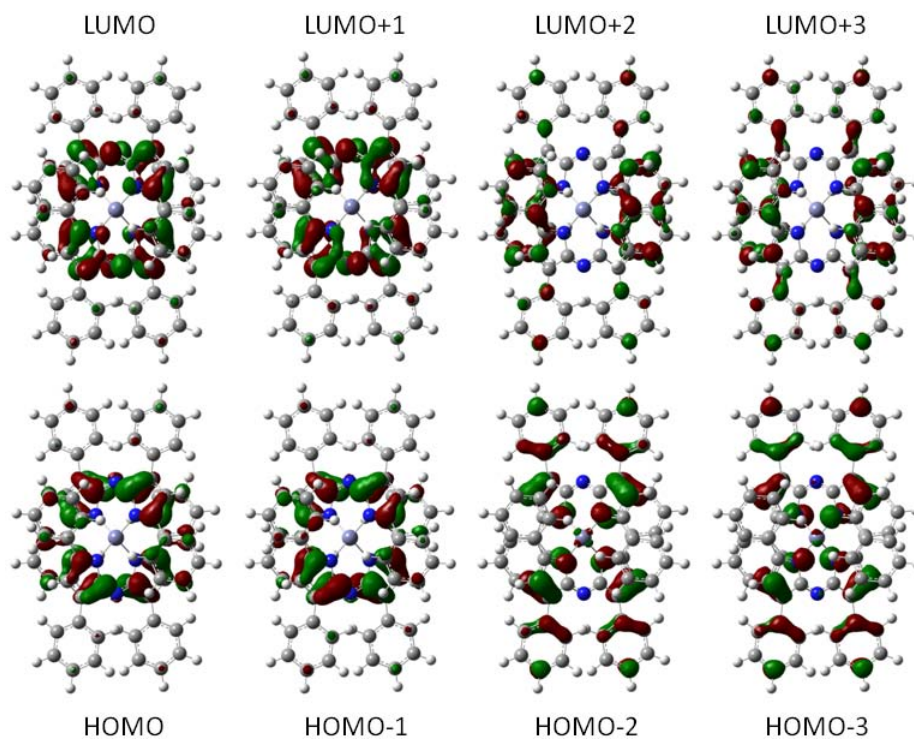


Figure S30: Calculated molecular orbital for ADP₂Zn.

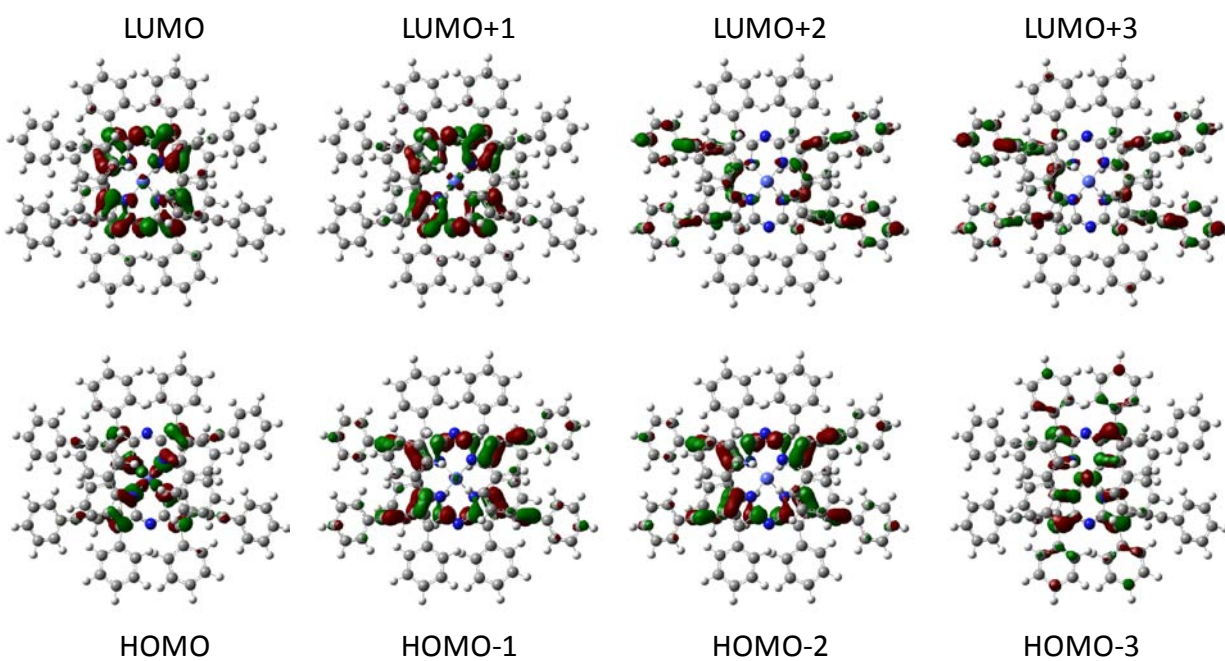


Figure S31: Calculated molecular orbital for WS₁₂Co.

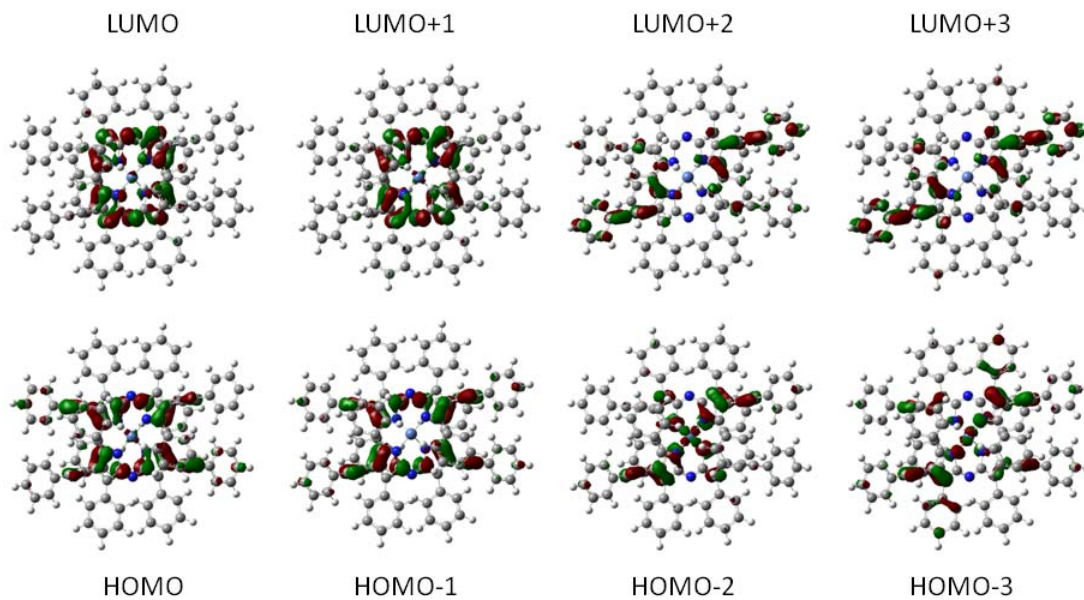


Figure S32: Calculated molecular orbital for WS₁₂Ni.

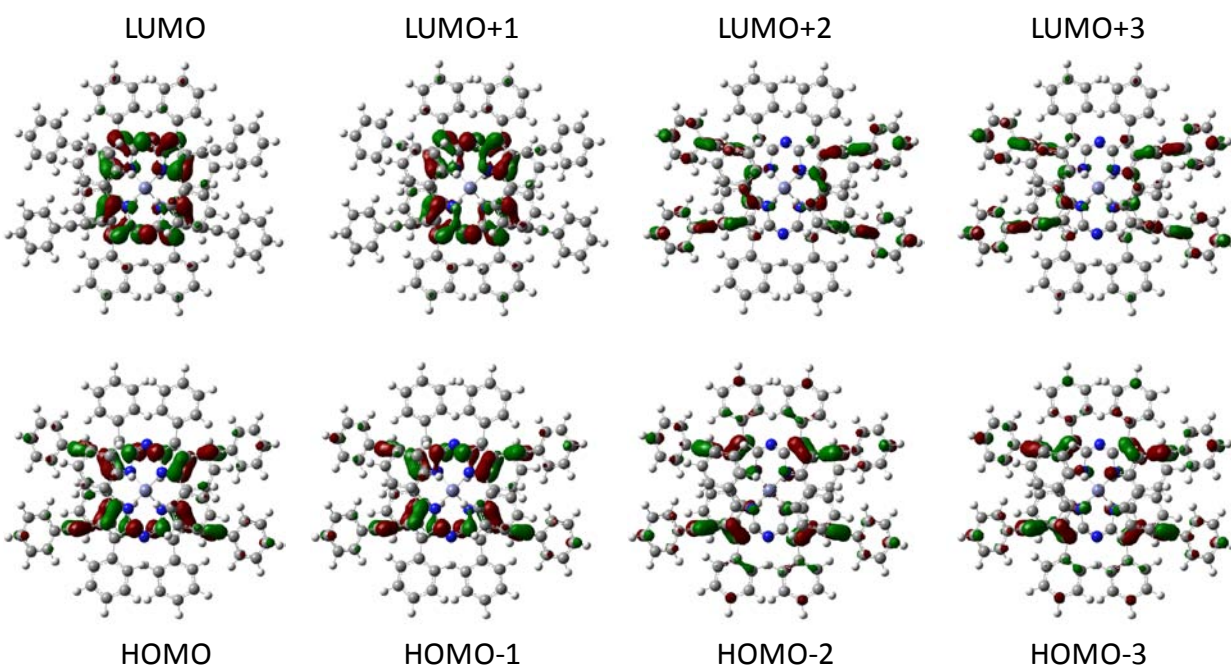


Figure S33: Calculated molecular orbital for WS₁₂Zn.

Table S3: Selected geometric parameters for ground state optimized geometries deduced from the pbepbe/6-31G(d,p) method^a

	Calculated	Experimental ^b	Calculated
	ADP ₂ Co		WS1 ₂ Co
M—N	1.959	1.979 (O'Shea 2009)	1.957
N—M—N	97.0/106.6/126.2	94.22/102-106/130.92 (O'Shea 2009)	97.1/106.1/126.7
	ADP ₂ Ni		WS1 ₂ Ni
M—N	1.948	1.968(O'Shea 2009)	1.945
N—M—N	95.0/105.3/138.9	92.81/102-106/131.8(O'Shea 2009)	95.2/104.8/140.3
	ADP ₂ Zn		WS1 ₂ Zn
M—N	1.992	1.987(O'Shea 2009) 1.985(Gray 2008)	1.991
N—M—N	96.5/108.9/124.3	94.66/102-106/130.07(O'Shea 2009) 94.56(Gray 2008)	96.3/107.6/125.9

^aAll distances are in Å and the angles are in degrees, ^b from crystallographic data

References: Palma, A.; Gallagher, J. F.; Mueller-Bunz, H.; Wolowska, J.; McInnes, E. J. L.; O'Shea, D. F. *Dalton Trans.* **2009**, 273–279.

Teets, T. S.; Partyka, D. V.; Updegraff, J. B.; Gray, T. G. *Inorg. Chem.* **2008**, *47*, 2338–2346.

Table: S4: The box dimensions for ADP and WS1 metal complexes, as well as that of PCBM for comparison.

	a, Å	b, Å	c, Å	Size, (Å) ³
PCBM	13	13	8	1400
ADP ₂ Co	18	13	8	1800
ADP ₂ Ni	19	13	8	1800
ADP ₂ Zn	19	13	8	1800
WS1 ₂ Co	21	19	12	4700
WS1 ₂ Ni	21	19	13	5300
WS1 ₂ Zn	21	19	13	4800

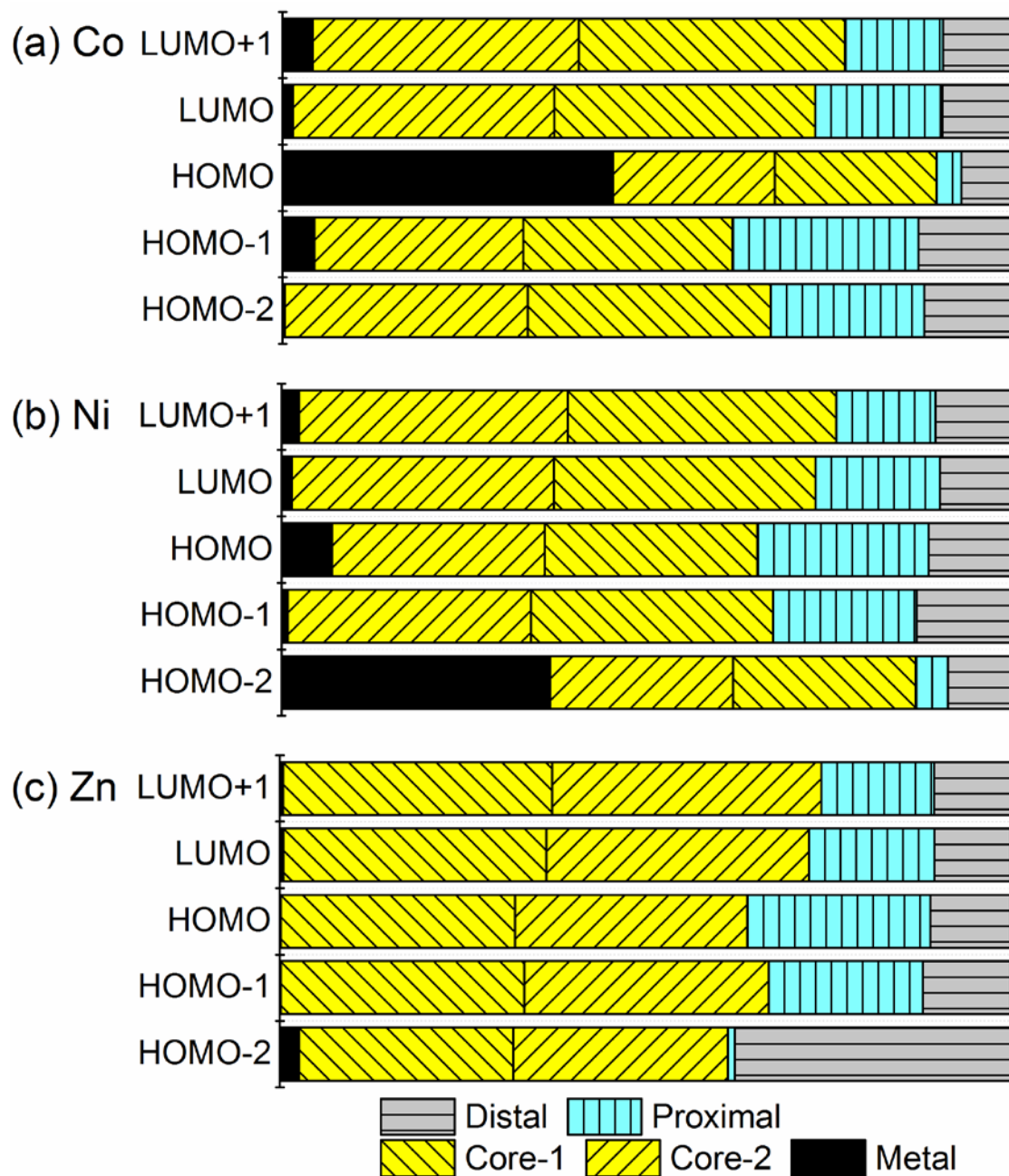


Figure S34: Estimated calculated contribution of different parts of ADP₂M complexes. (a) ADP₂Co; (b) ADP₂Ni; (c) ADP₂Zn

The optimized geometries in Cartesian coordinates (Å), energies (hartrees), frequencies (cm^{-1}) of WS1, WS1BF₂, WS1₂Co, WS1₂Ni, and WS1₂Zn using the pbepbe/6-31G(d,p) level of theory.

WS1-----

Electronic Energy (au): -2009.49472304
Sum of electronic and zero-point Energies (au): -2008.867920
Sum of electronic and thermal Energies (au): -2008.825682
Sum of electronic and thermal Enthalpies (au): -2008.824738
Sum of electronic and thermal Free Energies (au): -2008.950876

Optimized geometry

C1	3.415633	0.122610	0.012900
C2	2.463397	-0.945590	0.033479
C3	1.169468	-0.328797	0.033218
C4	-1.178550	-0.299409	0.032357
C5	-2.480349	-0.970140	0.060216
C6	-3.420311	0.073275	0.113845
C7	-2.639882	1.329283	0.110588
N8	1.362071	1.050571	0.003498
N9	-0.019949	-0.947425	0.038478
N10	-1.327893	1.091012	0.056124
C11	-3.161097	2.700107	0.140802
C12	-2.374343	3.754430	-0.382939
C13	-4.419892	3.011598	0.706451
C14	-2.836101	5.072283	-0.354075
H15	-1.404797	3.514364	-0.827116
C16	-4.874502	4.335002	0.740026
H17	-5.030027	2.215641	1.137708
C18	-4.089639	5.368678	0.207289
H19	-2.220062	5.873250	-0.773406
H20	-5.845480	4.560961	1.190730
H21	-4.450871	6.401017	0.230322
C22	2.726249	-2.388422	0.031775
C23	1.850923	-3.286993	0.691451
C24	3.856849	-2.921609	-0.633954
C25	2.102336	-4.663179	0.683852
H26	0.972449	-2.893299	1.205730
C27	4.102603	-4.299172	-0.636651
H28	4.531729	-2.249982	-1.168923
C29	3.229058	-5.177016	0.023405
H30	1.414390	-5.337855	1.202419
H31	4.977384	-4.689567	-1.165658
H32	3.424263	-6.253546	0.021658
C33	4.820478	0.005220	0.002762
C34	-4.820222	-0.032831	0.044315
C35	6.046891	-0.110243	-0.006649
C36	-6.046940	-0.131690	-0.042563
C37	-7.457827	-0.251958	-0.145861
C38	-8.067458	-1.532145	-0.217254
C39	-8.282505	0.902960	-0.180381
C40	-9.456700	-1.645934	-0.317987
H41	-7.434454	-2.423475	-0.195662
C42	-9.670516	0.774812	-0.281013
H43	-7.816435	1.890900	-0.130588
C44	-10.263387	-0.496605	-0.349871
H45	-9.914386	-2.638026	-0.373487
H46	-10.295114	1.672586	-0.307436
H47	-11.350098	-0.591341	-0.429758
C48	7.461238	-0.250241	-0.016722
C49	8.059094	-1.520959	0.186526

C50	8.297714	0.875831	-0.229819
C51	9.450571	-1.653796	0.176084
H52	7.416799	-2.390099	0.352874
C53	9.687816	0.729000	-0.236716
H54	7.840362	1.855963	-0.390734
C55	10.269940	-0.532832	-0.034356
H56	9.899621	-2.638702	0.334589
H57	10.322112	1.604832	-0.402222
H58	11.358162	-0.642278	-0.040925
C59	3.152650	2.744593	-0.018126
C60	4.416642	3.102357	0.509197
C61	2.329103	3.764292	-0.556441
C62	4.837247	4.436160	0.495708
H63	5.054840	2.331939	0.946097
C64	2.756984	5.094567	-0.566505
H65	1.362682	3.506443	-1.000374
C66	4.012857	5.437220	-0.040507
H67	5.813069	4.696693	0.915845
C68	2.111015	5.866597	-0.994203
H69	4.346473	6.478747	-0.049611
C70	2.685960	1.361284	0.004347
C71	-2.719832	-2.414509	0.041609
C72	-1.834208	-3.297655	-0.626360
C73	-3.847100	-2.969354	0.697915
C74	-2.072407	-4.676350	-0.636305
H75	-0.958671	-2.889540	-1.133848
C76	-4.079164	-4.348487	0.684187
H77	-4.529727	-2.309740	1.238612
C78	-3.194883	-5.209822	0.015525
H79	-1.376645	-5.337973	-1.161367
H80	-4.950931	-4.754419	1.206613
H81	-3.378748	-6.288313	0.004460
H82	0.528193	1.660172	0.058294

Frequencies (cm⁻¹):

9.9244	13.4403	15.6184
18.2434	18.7534	24.9292
28.1372	30.5752	36.3779
44.3151	45.4905	52.1258
55.5620	58.0872	61.9963
68.5060	77.1545	81.4850
102.9197	109.1225	121.9576
124.7838	134.2514	142.1662
170.4562	185.5026	202.8741
206.4511	216.0203	220.5628
227.6508	240.7983	248.2970
261.9435	287.1888	329.1619
333.7529	360.7398	362.9392
368.5868	382.3826	395.1666
395.3041	397.0101	398.3041
399.5684	400.5403	404.7923
437.9503	448.5556	459.4851
465.8922	474.7313	488.8376
495.9657	501.7669	506.9560
519.7442	532.3348	540.3475
574.3087	586.4783	592.9757
607.9022	609.6257	609.8271
610.2987	613.2363	613.6465
639.6996	647.8094	659.9354
670.6262	674.6121	678.4384
678.8953	679.7115	679.9557
680.8898	682.4254	683.0106

689.4547	700.7475	715.6851
737.2325	742.4259	743.1336
752.9208	755.2626	763.8420
766.5409	773.6802	790.1585
803.2896	818.0114	820.1837
821.3413	823.6961	824.4736
827.3119	831.3669	846.6130
892.6218	892.9095	893.4460
895.2335	896.5290	905.8756
933.1699	935.3454	937.4359
937.6946	938.5881	941.8771
956.7718	958.1250	962.5820
962.6419	964.7331	964.9455
967.4145	981.5980	981.8510
982.2183	983.7152	984.0048
984.5163	988.8211	1011.3476
1025.7614	1026.8772	1028.5833
1033.2540	1033.7948	1036.1913
1057.3126	1076.9235	1077.2130
1079.2180	1082.9443	1085.9935
1091.0639	1129.9950	1141.5658
1149.6045	1149.7332	1150.2717
1150.4482	1150.9645	1152.6454
1166.0373	1167.1477	1167.8686
1173.6323	1176.6228	1177.0391
1177.5389	1196.8852	1231.0951
1250.0381	1278.0302	1282.0202
1291.1036	1292.1426	1297.4337
1304.1715	1307.1934	1314.2661
1340.1848	1349.5583	1349.5829
1355.2510	1355.4274	1362.4857
1364.2343	1378.5607	1408.5484
1419.9775	1430.7572	1437.0385
1437.5255	1437.8495	1442.4671
1445.1354	1450.8130	1468.0666
1475.4624	1486.1392	1490.5870
1494.4760	1504.9091	1513.5773
1525.1581	1535.2142	1552.3114
1570.2059	1571.8299	1576.6083
1578.2561	1581.9174	1583.1856
1606.0721	1606.8407	1607.0818
1607.4458	1607.7336	1608.7593
2212.5838	2229.1055	3116.3893
3117.3908	3120.0717	3121.1375
3121.2393	3121.5283	3124.8301
3126.0675	3127.4815	3127.5916
3127.7326	3128.0220	3136.6407
3137.0803	3137.2331	3138.5593
3138.5917	3139.3521	3142.7158
3143.0241	3145.9868	3147.5214
3148.9324	3149.0074	3150.7911
3153.5617	3159.7444	3160.9002
3164.3711	3166.6540	3272.6440

WS1BF₂-----

Electronic Energy (au): -2233.39203838
Sum of electronic and zero-point Energies (au): -2232.763836
Sum of electronic and thermal Energies (au): -2232.719389
Sum of electronic and thermal Enthalpies (au): -2232.718445
Sum of electronic and thermal Free Energies (au): -2232.848244
Optimized geometry

B1	-0.003767	-1.719599	0.427707
F2	0.004299	-2.735039	-0.511720
F3	-0.016542	-2.209590	1.753312
C4	3.356673	0.099308	0.052582
C5	2.462859	1.196954	0.133847
C6	1.152001	0.614335	0.245141
C7	-1.156169	0.613919	0.269987
C8	-2.464417	1.199978	0.144173
C9	-3.354148	0.106622	-0.005989
C10	-2.570864	-1.109506	0.066323
N11	1.255251	-0.785075	0.257176
N12	-0.002069	1.274252	0.279972
N13	-1.258971	-0.784577	0.238350
C14	-3.105980	-2.472586	-0.008063
C15	-2.653685	-3.504443	0.848308
C16	-4.135719	-2.757156	-0.937907
C17	-3.222055	-4.779658	0.773479
H18	-1.869899	-3.292866	1.577504
C19	-4.687583	-4.039786	-1.014853
H20	-4.479683	-1.973977	-1.616747
C21	-4.237157	-5.054163	-0.155973
H22	-2.871076	-5.564867	1.449232
H23	-5.468280	-4.248767	-1.751983
H24	-4.674435	-6.055331	-0.212096
C25	2.776698	2.628283	0.119316
C26	1.871319	3.573730	-0.424987
C27	3.999574	3.101273	0.656464
C28	2.183594	4.937096	-0.430198
H29	0.924789	3.227149	-0.842979
C30	4.303347	4.466506	0.649607
H31	4.701290	2.391488	1.099649
C32	3.399236	5.391206	0.104348
H33	1.472861	5.649285	-0.860154
H34	5.248554	4.810984	1.079951
H35	3.640324	6.458319	0.096759
C36	4.758686	0.139045	-0.076426
C37	-4.759812	0.148580	-0.087733
C38	5.985000	0.173165	-0.187491
C39	-5.989783	0.183747	-0.144446
C40	-7.408029	0.220269	-0.215681
C41	-8.098674	1.459738	-0.203612
C42	-8.155223	-0.982933	-0.303501
C43	-9.493974	1.487796	-0.280096
H44	-7.525149	2.387842	-0.131430
C45	-9.550215	-0.940127	-0.379392
H46	-7.624567	-1.938972	-0.310234
C47	-10.224628	0.291697	-0.368441
H48	-10.015972	2.449073	-0.269475
H49	-10.116018	-1.873946	-0.446539
H50	-11.316424	0.319492	-0.427072
C51	7.398710	0.214908	-0.319275
C52	8.071131	1.455781	-0.466430
C53	8.159490	-0.982836	-0.305595

C54	9.462506	1.490487	-0.594271
H55	7.486154	2.379471	-0.480660
C56	9.550358	-0.933343	-0.435159
H57	7.642794	-1.939778	-0.191981
C58	10.206946	0.299734	-0.579096
H59	9.970321	2.452758	-0.707489
H60	10.126948	-1.862897	-0.423011
H61	11.295536	0.332572	-0.679742
C62	3.102742	-2.481224	0.079823
C63	4.138862	-2.786556	-0.835880
C64	2.640620	-3.495193	0.951839
C65	4.687844	-4.072081	-0.882953
H66	4.490649	-2.018315	-1.527487
C67	3.206069	-4.773257	0.906869
H68	1.849034	-3.268318	1.667766
C69	4.228282	-5.068439	-0.008096
H70	5.473746	-4.297114	-1.609762
H71	2.846673	-5.544225	1.594542
H72	4.663564	-6.071514	-0.040972
C73	2.570531	-1.114657	0.128112
C74	-2.768357	2.631026	0.151706
C75	-1.967814	3.541989	0.886267
C76	-3.870070	3.141658	-0.578446
C77	-2.261960	4.909215	0.886242
H78	-1.118097	3.165521	1.458543
C79	-4.157570	4.510229	-0.574029
H80	-4.486861	2.458931	-1.166995
C81	-3.357329	5.400589	0.158988
H82	-1.635025	5.594524	1.464398
H83	-5.007167	4.885059	-1.152703
H84	-3.586232	6.470356	0.163402

Frequencies (cm^{-1}):

9.9244	13.4403	15.6184
10.5371	11.3710	14.8237
16.5785	18.5785	26.0805
29.7411	35.2749	41.4687
42.7370	50.9176	54.1738
60.5421	65.7904	67.4250
69.7361	78.4615	82.2715
88.6978	107.1587	117.1998
123.4620	126.9973	148.8968
152.4140	173.1224	186.5831
188.9500	198.4193	211.0784
220.4160	229.1291	236.8806
240.5441	248.0974	262.8973
264.8303	281.2436	308.8701
330.4984	355.7088	362.2081
368.2921	375.0977	391.9228
394.8598	395.2751	396.9414
401.1689	402.6570	404.1646
421.8574	442.9297	448.9295
466.5776	477.3949	489.3973
496.3105	500.5596	501.1792
504.6694	514.9496	521.0512
536.9563	539.1006	563.5077
572.3990	589.9747	606.9249
607.3239	608.7878	609.3020
611.2500	612.7333	613.5302
637.8328	651.5156	661.6670
677.7987	679.0871	679.8749
679.9837	683.0362	684.0309

687.4805	688.9030	691.6692
705.9601	709.5065	723.2981
739.8327	743.4338	743.7184
752.9870	756.7796	757.3772
772.3321	787.7988	796.7464
819.1873	821.8790	824.9078
824.9158	833.1073	833.5972
840.7025	873.2057	895.2442
895.4998	896.3540	899.1344
913.8893	914.7857	936.0612
937.9900	938.7307	938.9828
950.2354	952.8089	959.4088
960.5066	961.5259	963.7400
963.9014	965.0811	976.2001
981.9856	982.0938	982.8558
982.9949	984.3451	984.6314
984.7780	990.7063	997.6099
1026.5165	1026.9828	1030.1754
1031.1663	1036.4974	1036.9939
1074.6436	1076.5728	1076.8784
1079.2794	1087.0150	1087.6937
1101.8989	1103.8902	1150.2679
1150.7552	1151.0606	1151.4947
1152.6925	1152.8596	1160.9377
1163.5403	1164.4010	1165.9121
1175.3569	1176.5219	1178.0316
1178.3678	1181.6477	1183.9715
1206.0185	1257.2892	1261.9173
1292.3180	1292.4999	1293.6507
1304.4518	1308.4322	1309.3931
1332.0268	1349.5167	1349.5821
1351.8813	1356.0169	1357.3867
1360.6629	1371.3942	1388.7855
1396.0272	1422.0977	1431.3338
1436.7001	1436.9638	1438.5089
1441.4591	1442.3295	1444.2730
1467.3696	1471.3507	1489.5158
1494.1127	1496.0485	1500.8721
1518.4732	1519.7117	1530.3002
1541.5973	1571.2057	1571.3358
1577.0062	1577.5633	1579.7014
1580.1856	1606.1425	1606.2516
1606.3808	1606.9787	1607.5373
1608.2248	2227.5265	2228.1245
3119.4668	3119.9447	3121.7654
3122.0949	3122.9350	3123.3017
3128.2905	3128.3939	3128.6928
3128.7938	3132.8106	3133.0562
3137.6440	3137.7929	3141.0511
3141.3715	3143.3568	3143.5408
3143.5733	3143.7911	3149.3284
3149.5600	3154.6358	3154.8549
3156.9102	3158.0213	3163.5567
3166.5003	3168.6463	3169.9570

WSI₂Co-----

Electronic Energy (au):			-5400.28466525
Sum of electronic and zero-point Energies=			-5399.052552
Sum of electronic and thermal Energies=			-5398.965205
Sum of electronic and thermal Enthalpies=			-5398.964261
Sum of electronic and thermal Free Energies=			-5399.197758
Optimized geometry			
C	0.83831200	-2.72094200	-0.67611900
N	1.10255900	-1.34995100	-0.85917200
N	-1.23967000	-1.24129000	0.89813800
C	-1.12871900	-2.62701000	0.67492500
N	-0.17795200	-3.25565600	-0.00811400
C	-2.39672200	-1.03424800	1.57446300
C	-3.08238600	-2.29186800	1.80546600
C	-2.26852100	-3.30795800	1.25345300
C	1.89484400	-3.50818200	-1.27980200
C	2.81951900	-2.57222600	-1.79783100
C	2.27776300	-1.25405000	-1.52735800
C	-0.83823400	2.72106600	-0.67616200
N	-1.10248600	1.35008400	-0.85927800
N	1.23947100	1.24133200	0.89833800
C	1.12873700	2.62704400	0.67494200
N	0.17804600	3.25574400	-0.00814800
C	2.39646800	1.03420100	1.57472500
C	3.08234000	2.29174300	1.80554400
C	2.26864700	3.30788700	1.25337800
C	-1.89477100	3.50833500	-1.27978900
C	-2.81945700	2.57240800	-1.79785300
C	-2.27770100	1.25421800	-1.52745300
C	2.82729600	-0.28899000	2.03398600
C	4.19838500	-0.63953100	2.03871800
C	1.88222500	-1.24257400	2.47872600
C	4.60407400	-1.90861100	2.46662300
H	4.93807100	0.08045500	1.68198500
C	2.29394100	-2.50730300	2.91129500
H	0.82199900	-0.97687600	2.50588500
C	3.65602900	-2.84633700	2.90498000
H	5.66632300	-2.16995600	2.44948500
H	1.54854200	-3.22867600	3.25869000
H	3.97669400	-3.83685300	3.24033000
C	2.52556300	4.74998900	1.24468100
C	1.46845100	5.68867400	1.33648700
C	3.85146600	5.24082200	1.15279400
C	1.73321500	7.06290800	1.34217500
H	0.44061100	5.32776400	1.40257000
C	4.10935900	6.61570700	1.15730900
H	4.67770200	4.53242200	1.05742900
C	3.05225800	7.53422100	1.25481300
H	0.90121800	7.76963400	1.41732100
H	5.14079600	6.97229500	1.07592600
H	3.25521600	8.60934400	1.26087800
C	-1.98180800	4.96959200	-1.32806500
C	-0.81990700	5.77416000	-1.43063300
C	-3.24218100	5.61610100	-1.28685300
C	-0.92009600	7.16834100	-1.49450900
H	0.15919100	5.29304600	-1.45878600
C	-3.33550300	7.01029700	-1.35021600
H	-4.14861500	5.01464900	-1.18600300
C	-2.17579700	7.79417300	-1.45685900
H	-0.00890000	7.76869300	-1.57587600

H	-4.31907800	7.48825300	-1.30784400
H	-2.25061000	8.88451200	-1.50868000
C	-2.86309400	-0.02427700	-1.94216600
C	-2.04644000	-1.07672300	-2.41621800
C	-4.26148400	-0.22824400	-1.86992100
C	-2.61026400	-2.29788000	-2.80119100
H	-0.96752900	-0.92292600	-2.50647500
C	-4.81881900	-1.45507000	-2.24782100
H	-4.90178800	0.57151800	-1.49111300
C	-3.99744400	-2.49325700	-2.71455300
H	-1.96331600	-3.09853300	-3.17130700
H	-5.89984400	-1.60420500	-2.16950400
H	-4.43632300	-3.45053400	-3.01029500
C	1.98188900	-4.96943500	-1.32815400
C	3.24227300	-5.61593300	-1.28705200
C	0.81999500	-5.77401600	-1.43070300
C	3.33561000	-7.01012300	-1.35049100
H	4.14870700	-5.01447800	-1.18622500
C	0.92019900	-7.16819200	-1.49465500
H	-0.15911200	-5.29291500	-1.45877900
C	2.17591000	-7.79401100	-1.45710700
H	4.31919500	-7.48806600	-1.30820200
H	0.00900500	-7.76854900	-1.57600000
H	2.25073400	-8.88434700	-1.50899200
C	2.86319600	0.02446000	-1.94197600
C	2.04658700	1.07694200	-2.41602400
C	4.26158600	0.22840000	-1.86964900
C	2.61045300	2.29810500	-2.80091600
H	0.96767800	0.92316800	-2.50634300
C	4.81896200	1.45523300	-2.24746400
H	4.90185800	-0.57139000	-1.49084700
C	3.99763100	2.49345500	-2.71419600
H	1.96353800	3.09878600	-3.17102900
H	5.89986000	1.60434500	-2.16908100
H	4.43654300	3.45073800	-3.00987300
C	-2.82782500	0.28894300	2.03345800
C	-1.88296200	1.24281000	2.47803800
C	-4.19898200	0.63921600	2.03805300
C	-2.29494500	2.50754800	2.91032500
H	-0.82268100	0.97733200	2.50529100
C	-4.60494000	1.90830600	2.46567500
H	-4.93850900	-0.08098800	1.68143100
C	-3.65710000	2.84631100	2.90388100
H	-1.54970200	3.22914300	3.25759400
H	-5.66724000	2.16943600	2.44843400
H	-3.97797700	3.83683300	3.23900800
C	-2.52520800	-4.75010100	1.24494600
C	-1.46795300	-5.68860700	1.33694600
C	-3.85102800	-5.24115500	1.15305400
C	-1.73250200	-7.06288200	1.34280100
H	-0.44017300	-5.32752800	1.40305200
C	-4.10870600	-6.61607900	1.15773400
H	-4.67736900	-4.53289200	1.05755900
C	-3.05146500	-7.53441300	1.25541700
H	-0.90040100	-7.76946900	1.41809300
H	-5.14008400	-6.97283900	1.07634000
H	-3.25425400	-8.60956700	1.26161300
C	-4.26085900	-2.44995400	2.55987300
C	3.97887700	-2.82480900	-2.55607500
C	4.98791000	-3.02623600	-3.23451100
C	-5.28342100	-2.58871300	3.23370800

C	6.15251500	-3.25266800	-4.01554400
C	6.57207200	-4.57293300	-4.32372100
C	6.91692200	-2.15932000	-4.50031300
C	7.72084800	-4.78586900	-5.09102400
H	5.98318200	-5.41719700	-3.95491000
C	8.06384600	-2.38650900	-5.26617700
H	6.59385200	-1.14088400	-4.26738400
C	8.47087300	-3.69709700	-5.56480900
H	8.03320000	-5.80844300	-5.32269400
H	8.64413100	-1.53538600	-5.63465300
H	9.36841300	-3.86918500	-6.16576100
C	-6.46298500	-2.75326000	4.00782800
C	-6.99944800	-4.04702000	4.23791700
C	-7.12569100	-1.62756700	4.56278400
C	-8.16235300	-4.20253300	4.99756100
H	-6.48876900	-4.91653500	3.81505900
C	-8.28797100	-1.79734200	5.32041500
H	-6.71268900	-0.62977200	4.39069700
C	-8.81131200	-3.08183600	5.54103700
H	-8.56524800	-5.20522600	5.16841800
H	-8.78913700	-0.92170300	5.74347000
H	-9.72043600	-3.20909500	6.13569200
C	4.26083200	2.44973100	2.55994200
C	5.28340700	2.58840300	3.23377500
C	6.46300600	2.75281200	4.00787000
C	6.99972800	4.04649600	4.23779000
C	7.12549200	1.62705900	4.56296500
C	8.16267000	4.20187400	4.99740200
H	6.48921700	4.91605800	3.81482400
C	8.28781400	1.79669900	5.32056300
H	6.71228900	0.62932400	4.39101100
C	8.81141300	3.08111800	5.54101500
H	8.56576800	5.20450900	5.16812600
H	8.78880900	0.92101600	5.74372600
H	9.72056800	3.20827200	6.13564500
C	-3.97883700	2.82504200	-2.55604800
C	-4.98789400	3.02651100	-3.23443700
C	-6.15253500	3.25295600	-4.01541200
C	-6.57215300	4.57322600	-4.32347600
C	-6.91691900	2.15961300	-4.50023200
C	-7.72096500	4.78617500	-5.09072300
H	-5.98328300	5.41748500	-3.95462200
C	-8.06387800	2.38681400	-5.26603900
H	-6.59380200	1.14117300	-4.26738800
C	-8.47096500	3.69740900	-5.56456100
H	-8.03336400	5.80875400	-5.32230600
H	-8.64414500	1.53569600	-5.63455600
H	-9.36853300	3.86950800	-6.16546900
Co	-0.00005200	0.00003900	0.02913800

Frequencies (cm⁻¹):

6.1364	6.1495	8.5514
9.6947	10.3835	10.6268
12.2931	13.8106	18.2814
19.2205	19.6671	21.0549
23.7718	23.8955	26.4870
27.4880	27.9974	28.0545
32.7449	39.9439	42.1548
44.1619	47.4022	49.7881
49.9195	51.4458	53.1539
55.1460	56.5115	58.7059
60.9954	63.4297	65.7029

66.9994	71.8865	71.9053
76.3979	77.2199	77.9079
79.2132	100.8080	101.0497
105.6800	109.1559	110.8423
116.8986	117.6733	118.2757
131.0953	138.4013	139.8065
142.5098	145.6865	150.9185
166.7774	188.0698	191.7011
195.5435	199.6580	203.6734
208.5382	212.1180	212.7736
216.0115	218.6347	226.0278
227.3113	227.3458	228.6255
234.6017	240.8731	243.2102
261.2874	266.9282	269.2541
286.6573	296.8181	313.8333
321.5082	334.0778	334.2690
339.7355	341.7059	354.0880
354.7113	361.5818	361.7821
378.8593	384.7772	387.4445
393.2901	395.1651	395.1658
395.4535	395.4553	397.2976
398.2023	398.6046	399.4707
399.9882	400.4953	404.6371
405.1254	417.8745	418.5075
439.1226	441.2706	443.7498
448.7730	465.9176	466.0346
480.6363	483.8019	488.4080
489.9962	496.5579	496.6195
496.9768	497.1519	502.2654
502.9761	504.0289	504.2321
517.8383	518.8308	534.2901
534.2922	539.5139	539.5293
566.4209	566.7374	591.7290
591.7335	595.7690	596.8533
608.0204	608.3421	608.5691
608.8445	608.8983	609.1897
609.5753	609.5776	613.1065
613.1089	613.4134	613.4178
641.6359	642.9469	661.0605
661.1163	664.3307	666.8080
670.2578	671.3760	677.5788
678.3681	678.4533	679.3960
679.8900	679.9801	680.2632
680.3110	680.5651	680.5765
680.8567	680.8590	684.9004
685.3705	688.8690	689.1883
703.3973	703.4753	706.6075
706.6469	713.1107	713.5676
735.6126	735.8685	742.8482
742.8663	743.0904	743.1015
755.3986	755.4336	756.2275
756.3204	758.1933	758.5303
767.8889	767.9848	793.0680
793.0799	813.2059	813.7789
814.3113	815.5629	816.5107
817.3063	818.1876	820.3090
821.3941	821.4955	824.6282
824.6330	824.7544	824.7721
840.2499	840.2884	868.4458
868.7483	889.6792	891.4107
892.5754	892.7542	892.8115

893.3060	893.3242	893.3677
893.4909	894.7301	895.0061
895.4408	931.5872	931.6338
932.8428	934.2503	934.5426
934.6524	934.8670	936.1998
937.7186	937.7196	937.9441
937.9444	954.9245	954.9268
956.7057	956.7214	959.6639
960.0537	960.3496	960.7921
962.2546	962.2562	962.5500
962.5513	973.1987	973.5889
976.9821	977.6171	981.8140
981.8149	981.9146	981.9152
982.8753	983.2342	983.2979
983.6875	984.3879	984.4555
984.7969	984.8887	1018.5681
1019.7698	1025.2575	1025.2622
1026.6234	1026.9803	1027.2692
1027.9369	1033.0205	1033.1816
1033.5294	1033.7476	1039.1009
1040.4978	1055.4574	1055.5528
1076.2572	1076.2584	1076.5393
1076.5404	1079.5186	1080.1197
1082.2948	1083.6462	1085.0342
1085.1279	1089.3959	1089.5116
1149.2089	1149.2231	1149.5548
1149.5772	1149.7994	1149.8017
1149.8831	1149.8856	1150.5598
1150.8496	1151.0026	1151.1267
1151.6525	1151.7507	1157.3533
1157.5153	1158.3162	1159.0413
1167.9081	1168.5907	1168.6890
1169.7041	1170.0215	1171.0056
1171.3008	1172.6517	1174.0845
1174.1657	1174.9501	1174.9986
1179.7715	1180.3031	1250.8370
1251.1407	1252.3666	1253.1253
1269.7356	1271.7782	1288.1294
1290.8830	1291.4775	1291.4940
1291.5703	1291.9061	1300.6631
1300.7455	1305.7432	1305.7673
1310.2146	1311.6999	1328.3925
1333.1814	1349.1470	1349.1473
1349.1575	1349.1595	1354.9934
1355.0039	1355.5795	1355.6164
1359.8092	1359.9354	1360.7325
1361.6402	1377.5500	1378.1404
1388.2546	1388.3012	1414.3744
1415.1945	1421.0932	1421.8962
1431.6695	1431.8998	1435.7145
1435.7241	1437.2021	1437.2055
1437.3480	1437.3649	1439.9290
1440.0070	1440.3193	1440.6407
1464.8966	1465.1587	1467.1901
1467.1981	1474.9980	1476.0055
1492.4734	1492.6268	1494.2351
1494.8701	1495.0092	1495.4138
1500.5420	1501.7791	1520.5723
1520.6820	1522.4838	1522.6106
1556.6391	1557.5860	1570.8092
1570.8094	1570.8199	1570.8201

1576.7004	1576.7590	1577.0044
1577.0944	1580.0352	1580.1882
1580.8035	1580.9176	1604.6115
1604.8916	1605.6988	1605.7253
1605.7273	1605.9552	1606.5581
1606.5649	1606.6737	1606.7338
1607.1997	1607.2049	2222.6307
2222.8317	2223.3830	2223.3892
3116.6752	3116.6769	3117.0882
3117.0930	3120.1973	3120.1994
3120.2392	3120.2427	3121.1160
3121.2122	3121.5430	3121.8756
3125.3923	3125.3944	3126.2441
3126.2444	3126.8499	3126.8506
3126.9434	3126.9459	3128.0356
3128.1316	3128.4112	3129.1037
3136.3553	3136.3598	3136.4704
3136.4784	3136.6681	3136.7124
3137.4205	3138.2318	3138.6049
3138.6079	3138.9399	3138.9683
3142.1280	3142.1310	3142.2834
3142.2869	3145.4476	3145.6505
3145.8731	3146.1412	3148.1093
3148.1136	3148.1881	3148.2011
3149.7641	3149.7666	3151.0928
3151.1041	3154.2260	3154.2421
3154.8571	3154.9113	3164.0032
3164.0072	3164.6766	3164.6830

WSI₂Ni-----

Electronic Energy (au):			-5525.78152372
Sum of electronic and zero-point Energies=			-5524.548692
Sum of electronic and thermal Energies=			-5524.461695
Sum of electronic and thermal Enthalpies=			-5524.460751
Sum of electronic and thermal Free Energies=			-5524.689577
Optimized geometry			
C	-0.54470700	-2.74772500	0.63072100
N	-0.92168200	-1.39450800	0.74612300
N	1.41067600	-1.16336200	-0.91749000
C	1.42760700	-2.54321200	-0.67967900
N	0.51933300	-3.23361800	0.00199200
C	2.54831700	-0.85570300	-1.58522300
C	3.34763000	-2.04736900	-1.80172200
C	2.62623700	-3.12890200	-1.24209400
C	-1.53331300	-3.58868900	1.27557200
C	-2.52332500	-2.70649900	1.76320400
C	-2.08711500	-1.36134400	1.43476300
C	0.54469100	2.74780800	0.63066000
N	0.92159400	1.39458600	0.74621600
N	-1.41060800	1.16333000	-0.91756200
C	-1.42757400	2.54319600	-0.67979400
N	-0.51933300	3.23365500	0.00186200
C	-2.54824100	0.85562400	-1.58527300
C	-3.34759800	2.04726400	-1.80179800
C	-2.62622800	3.12883200	-1.24222400
C	1.53332200	3.58879100	1.27543500
C	2.52330200	2.70660400	1.76315300
C	2.08703600	1.36144000	1.43484800
C	-2.85282400	-0.50115700	-2.04615800
C	-4.18084100	-0.98911200	-2.04629900
C	-1.81803800	-1.35544800	-2.49373000
C	-4.45600900	-2.29430400	-2.46988400
H	-4.98888000	-0.34704800	-1.68925500
C	-2.09807500	-2.65766400	-2.91959900
H	-0.79042200	-0.98047500	-2.53539400
C	-3.41888200	-3.13291400	-2.90739300
H	-5.48612900	-2.66220500	-2.44968600
H	-1.28425100	-3.29993000	-3.26839200
H	-3.63822600	-4.15210300	-3.23815700
C	-3.00013500	4.54448100	-1.22859700
C	-2.01955800	5.56546100	-1.29392900
C	-4.36230500	4.92801900	-1.15503700
C	-2.39166100	6.91433700	-1.28988300
H	-0.96556000	5.28752300	-1.34736900
C	-4.72751400	6.27827900	-1.15062900
H	-5.13173800	4.15612300	-1.08011500
C	-3.74519900	7.27876600	-1.22073600
H	-1.61705100	7.68530000	-1.34426000
H	-5.78512500	6.55159600	-1.08377800
H	-4.03305800	8.33436100	-1.21994000
C	1.50569500	5.04946600	1.38393800
C	0.28448400	5.75755500	1.50872300
C	2.71242400	5.79233800	1.37956300
C	0.27645400	7.15182600	1.62655700
H	-0.65446900	5.20156700	1.51064200
C	2.69738400	7.18612100	1.49777600
H	3.66331700	5.26709000	1.26376200
C	1.48004500	7.87370600	1.62344500
H	-0.67881800	7.67662200	1.72379900

H	3.64143700	7.73948100	1.48339400
H	1.46996800	8.96375000	1.71730000
C	2.77061200	0.12960800	1.84703800
C	2.05135700	-0.95613200	2.39522200
C	4.17619500	0.02439300	1.72540900
C	2.71892000	-2.11605600	2.80437500
H	0.96890600	-0.87658800	2.52134200
C	4.83663300	-1.14337700	2.12381200
H	4.74028000	0.85300900	1.29095100
C	4.11177900	-2.21635300	2.66580300
H	2.14805500	-2.94455100	3.23380700
H	5.92170600	-1.21813000	2.00515800
H	4.63032300	-3.12694000	2.97959600
C	-1.50562700	-5.04935400	1.38419900
C	-2.71232400	-5.79227800	1.37982000
C	-0.28439000	-5.75737600	1.50910400
C	-2.69722800	-7.18605100	1.49814200
H	-3.66323300	-5.26707800	1.26392900
C	-0.27630500	-7.15163700	1.62704700
H	0.65453600	-5.20134300	1.51103000
C	-1.47986400	-7.87357000	1.62392700
H	-3.64125500	-7.73945500	1.48375100
H	0.67898500	-7.67638500	1.72437900
H	-1.46974200	-8.96360700	1.71786600
C	-2.77074500	-0.12951700	1.84687500
C	-2.05152700	0.95633700	2.39488500
C	-4.17634900	-0.02442200	1.72537700
C	-2.71914200	2.11624300	2.80400200
H	-0.96905400	0.87690300	2.52088700
C	-4.83684300	1.14332700	2.12375000
H	-4.74041600	-0.85311800	1.29104800
C	-4.11202500	2.21641200	2.66557300
H	-2.14829600	2.94482500	3.23328900
H	-5.92193400	1.21797500	2.00519900
H	-4.63061200	3.12698400	2.97933900
C	2.85294200	0.50107400	-2.04608300
C	1.81817300	1.35542300	-2.49358300
C	4.18097800	0.98898000	-2.04625200
C	2.09824100	2.65764800	-2.91940400
H	0.79054100	0.98049000	-2.53522800
C	4.45617800	2.29417900	-2.46979500
H	4.98900700	0.34687200	-1.68926400
C	3.41906600	3.13284800	-2.90722800
H	1.28442600	3.29995800	-3.26813500
H	5.48631300	2.66204000	-2.44962000
H	3.63843700	4.15204300	-3.23795500
C	3.00011000	-4.54455700	-1.22841400
C	2.01950600	-5.56551800	-1.29365600
C	4.36227300	-4.92812400	-1.15487600
C	2.39157800	-6.91440300	-1.28955000
H	0.96551300	-5.28755700	-1.34707500
C	4.72745000	-6.27839200	-1.15040800
H	5.13172700	-4.15624200	-1.08001800
C	3.74510900	-7.27886000	-1.22043000
H	1.61694700	-7.68535000	-1.34385700
H	5.78505800	-6.55173000	-1.08357600
H	4.03294300	-8.33446200	-1.21958700
Ni	0.00006200	0.00002000	-0.25069900
C	4.54123800	-2.09856300	-2.54631000
C	-3.65767100	-3.01202300	2.53876800
C	-4.64913700	-3.25701800	3.22867700

C	5.57843600	-2.13595500	-3.21132200
C	-5.79637700	-3.53126400	4.01973400
C	-6.12962600	-4.86396700	4.37599800
C	-6.63123400	-2.47304000	4.46468200
C	-7.26391400	-5.12322600	5.15060700
H	-5.48633000	-5.68100000	4.03797700
C	-7.76264500	-2.74650400	5.23846000
H	-6.37465600	-1.44503400	4.19394100
C	-8.08445000	-4.06916700	5.58430400
H	-7.50961400	-6.15490200	5.41928800
H	-8.39790200	-1.92215400	5.57583700
H	-8.97039300	-4.27747300	6.19099000
C	6.77670700	-2.17989100	-3.97268300
C	7.46076400	-3.40743300	-4.17181300
C	7.31193100	-0.99614300	-4.54439000
C	8.64294800	-3.44209600	-4.91672300
H	7.04848700	-4.32200000	-3.73679600
C	8.49481900	-1.04506100	-5.28734600
H	6.78516200	-0.04941800	-4.39611800
C	9.16514700	-2.26462100	-5.47650100
H	9.16062000	-4.39467100	-5.06336800
H	8.89669200	-0.12562900	-5.72327000
H	10.09001300	-2.29768100	-6.05946300
C	-4.54121600	2.09839800	-2.54637400
C	-5.57843500	2.13572900	-3.21135600
C	-6.77671400	2.17955800	-3.97271200
C	-7.46084400	3.40704900	-4.17189600
C	-7.31187000	0.99575100	-4.54435900
C	-8.64303400	3.44160600	-4.91680100
H	-7.04861900	4.32166200	-3.73692700
C	-8.49476500	1.04456300	-5.28731100
H	-6.78504300	0.04906500	-4.39604500
C	-9.16516700	2.26407400	-5.47652000
H	-9.16076300	4.39414500	-5.06348900
H	-8.89658600	0.12508700	-5.72318900
H	-10.09003700	2.29705200	-6.05947900
C	3.65765700	3.01212800	2.53870400
C	4.64913900	3.25713300	3.22858700
C	5.79635000	3.53151000	4.01964100
C	6.12954800	4.86426700	4.37575000
C	6.63122400	2.47336600	4.46474500
C	7.26380100	5.12365600	5.15036600
H	5.48624000	5.68123900	4.03760800
C	7.76260000	2.74695900	5.23852800
H	6.37468500	1.44531800	4.19412200
C	8.08435300	4.06967300	5.58422200
H	7.50946200	6.15537200	5.41893000
H	8.39787000	1.92266800	5.57602800
H	8.97026800	4.27808000	6.19091400

Frequencies (cm⁻¹):

7.5899	9.1121	10.5463
10.7015	13.7567	14.1478
15.2052	16.0693	19.7910
21.0948	21.1265	22.3747
28.1665	28.6831	31.0251
31.1080	31.9231	32.0771
36.1949	44.6451	45.0422
49.9269	51.3660	51.8985
52.6360	55.5028	57.3196
58.6949	61.9541	64.2203
64.3912	67.1950	71.2328

74.1287	74.7115	76.8406
78.9631	79.0108	79.2525
81.2716	99.0567	102.5077
106.5733	110.7070	111.4947
116.2748	117.2215	120.1637
132.1151	139.4269	141.0920
142.3246	146.5635	152.0384
168.7721	186.7732	192.0618
193.4883	199.4265	204.9009
208.2289	213.2204	213.5751
216.0314	218.2998	225.9809
226.9955	227.0767	228.5918
233.9505	239.3752	242.3128
264.5539	265.1223	270.3780
285.2318	293.2623	312.9058
322.4170	334.0094	334.2675
339.4847	340.3815	353.1354
354.5556	362.5788	362.8308
380.2392	386.0920	387.3513
391.6177	395.5917	395.5928
395.9049	395.9051	399.1435
399.3176	399.8072	401.3995
401.6931	402.5482	404.7501
405.8452	415.9635	417.7288
440.4812	442.1926	446.5405
450.6968	467.3926	468.0119
480.9799	483.3108	488.8680
489.6565	496.8726	496.8956
498.0287	498.1880	503.4100
503.6159	504.2309	504.4783
518.3411	518.5187	535.7561
535.7765	540.8318	540.9348
566.2953	566.8050	591.2241
591.2484	596.5565	597.5358
608.0363	608.3070	608.6031
609.0800	609.1291	609.3070
610.1184	610.1314	613.2401
613.2414	613.4261	613.4317
642.9460	643.5645	661.4049
661.6017	663.7550	665.8567
670.3087	670.3907	678.7461
678.8859	680.0159	680.2113
680.5392	680.5711	680.6158
680.8520	681.3288	682.6529
683.7492	683.9574	685.3767
686.0353	689.5611	690.0830
704.0389	705.4266	706.6224
707.4202	713.2027	714.0055
734.8329	734.8481	742.5910
742.6046	743.1357	743.1541
754.7066	755.2736	756.0819
756.5802	758.3823	758.6422
768.3748	768.3973	792.9650
792.9928	817.1546	817.6101
817.8311	818.0725	818.1265
819.8263	821.2939	822.3358
822.6309	824.0399	824.4535
824.5020	825.1855	825.3791
841.0873	842.6809	867.2073
868.1841	892.9528	893.0510
893.2069	893.4359	893.6098

893.7520	893.8294	895.1568
895.3449	895.4470	896.5009
899.2960	932.5225	932.5266
934.6229	935.4800	935.6721
936.3130	936.5486	937.5727
937.5737	938.2007	938.2023
938.5504	955.7964	955.8003
957.7513	957.7835	959.7918
960.4600	960.9697	961.4287
962.1145	962.1157	962.5125
962.5146	972.5156	972.8336
979.6903	980.2086	981.9318
981.9374	981.9734	981.9742
983.0127	983.2909	983.4008
983.7813	984.5198	984.8868
985.6222	985.7888	1019.0956
1020.8691	1025.4916	1025.5367
1026.4604	1026.9124	1027.4844
1027.8611	1033.1692	1033.3383
1034.4851	1034.9043	1040.3623
1042.2626	1056.8362	1058.0041
1076.1489	1076.1503	1076.4872
1076.4880	1079.1808	1081.1257
1081.5049	1084.0070	1085.2509
1085.3188	1090.3733	1091.1401
1149.2832	1149.3691	1149.7870
1149.8626	1149.8851	1149.8931
1150.0590	1150.0615	1150.1318
1150.6891	1151.0503	1151.1539
1151.4479	1151.7991	1156.5221
1156.6298	1160.0093	1160.4777
1167.2784	1168.5423	1168.7236
1169.8229	1170.5499	1171.1274
1172.0251	1172.4802	1174.2337
1174.2346	1175.2112	1175.2818
1186.8468	1186.9067	1250.7053
1251.5303	1253.6581	1254.4261
1270.6180	1271.9429	1289.2083
1291.0825	1291.2564	1291.3450
1291.5256	1292.3599	1300.8901
1300.9012	1305.7920	1305.8656
1310.0140	1310.8069	1331.4192
1336.6414	1349.2117	1349.2139
1349.2538	1349.2555	1355.0184
1355.0427	1355.9656	1355.9844
1358.7428	1358.8968	1360.8865
1361.6315	1378.6350	1379.4431
1387.9638	1388.1568	1414.6909
1415.8334	1422.4296	1423.7852
1432.9587	1433.2291	1435.9105
1435.9918	1437.3253	1437.3308
1437.4416	1437.4442	1439.6845
1439.8378	1440.7306	1440.8953
1465.2559	1465.7764	1467.3287
1467.3512	1477.6065	1477.6651
1492.4784	1492.6400	1493.9970
1494.8153	1495.5719	1495.7800
1502.0997	1503.3530	1520.7500
1520.7762	1523.1363	1523.4026
1557.5489	1558.3937	1570.7855
1570.7856	1570.8762	1570.8766

1576.7663	1576.7684	1577.0606
1577.2190	1579.5141	1580.2375
1580.6424	1581.3392	1604.8334
1605.0610	1605.7147	1605.7688
1606.1862	1606.4566	1606.6068
1606.6312	1606.8063	1606.8261
1607.5815	1607.5855	2221.5566
2221.6161	2222.7361	2222.7495
3111.4371	3112.6880	3116.4717
3116.4733	3116.8371	3116.8436
3120.4894	3120.4918	3120.7503
3120.7529	3120.9010	3120.9421
3124.1329	3124.2087	3125.1481
3125.1503	3125.9331	3125.9342
3127.1326	3127.1332	3127.1601
3127.1605	3128.8872	3128.9970
3133.5934	3133.6369	3136.7244
3136.7269	3136.9631	3136.9653
3138.5296	3138.5302	3138.8201
3138.8525	3140.8556	3141.0706
3142.4009	3142.4041	3142.4688
3142.4711	3145.4650	3145.4735
3148.4259	3148.4336	3148.6295
3148.6416	3149.7777	3150.3898
3150.5844	3150.5881	3150.8727
3150.8798	3152.5462	3152.7217
3156.4564	3156.4792	3164.3149
3164.3175	3165.5563	3165.5592

WSI₂Zn-----

Electronic Energy (au):			-5796.73334410
Sum of electronic and zero-point Energies=			-5795.500361
Sum of electronic and thermal Energies=			-5795.413014
Sum of electronic and thermal Enthalpies=			-5795.412070
Sum of electronic and thermal Free Energies=			-5795.643283
Optimized geometry			
C	2.32054100	1.18664500	1.60527800
C	2.91013200	2.48411600	1.88404400
C	2.03838100	3.45197900	1.33551600
C	0.96800000	2.70264600	0.70785200
C	-0.96678000	2.70301500	-0.70830700
C	-2.03687500	3.45277000	-1.33597200
C	-2.90918100	2.48522400	-1.88418500
C	-2.32015800	1.18752400	-1.60530400
N	1.16888700	1.32729500	0.91359700
N	0.00076300	3.27815900	-0.00028900
N	-1.16833800	1.32772400	-0.91381600
C	2.84995100	-0.11538600	2.02412700
C	1.98535100	-1.14490700	2.46166700
C	4.24218500	-0.36576500	1.98942400
C	2.49624300	-2.38956400	2.84541400
H	0.91014300	-0.95684700	2.52802200
C	4.74700300	-1.61456500	2.36875600
H	4.91957700	0.41618900	1.63904700
C	3.87804800	-2.63006100	2.79764600
H	1.81228400	-3.17184200	3.18724600
H	5.82437400	-1.79870800	2.32116200
H	4.27606900	-3.60461800	3.09473200
C	-2.85027700	-0.11430200	-2.02390500
C	-1.98630500	-1.14416800	-2.46186500
C	-4.24259900	-0.36409300	-1.98856800
C	-2.49789600	-2.38861600	-2.84537200
H	-0.91105700	-0.95653200	-2.52876900
C	-4.74811400	-1.61268500	-2.36766000
H	-4.91950100	0.41815300	-1.63789000
C	-3.87977500	-2.62854500	-2.79694300
H	-1.81442200	-3.17117400	-3.18753100
H	-5.82554000	-1.79637900	-2.31957000
H	-4.27833800	-3.60294100	-3.09383000
C	-2.17827400	4.91038500	-1.37913700
C	-1.04508100	5.75695500	-1.45759500
C	-3.46193200	5.50971000	-1.35806900
C	-1.19511900	7.14694300	-1.51688600
H	-0.04861100	5.31211000	-1.47029100
C	-3.60540200	6.89996100	-1.41667200
H	-4.34697600	4.87419900	-1.27712400
C	-2.47336400	7.72610500	-1.49897400
H	-0.30541100	7.78085600	-1.57874100
H	-4.60644200	7.34137100	-1.39007400
H	-2.58700000	8.81326000	-1.54735000
C	2.18051300	4.90953200	1.37839900
C	1.04774700	5.75668300	1.45668800
C	3.46447200	5.50820000	1.35719500
C	1.19848700	7.14660800	1.51568000
H	0.05105000	5.31234400	1.46949300
C	3.60864600	6.89839200	1.41549800
H	4.34918900	4.87221400	1.27637200
C	2.47702300	7.72512300	1.49763100
H	0.30909900	7.78098200	1.57740600

H	4.60991000	7.33928800	1.38879400
H	2.59120300	8.81223000	1.54577200
C	4.05923900	2.69783000	2.66955100
C	5.05745300	2.87248100	3.37088000
C	6.20956500	3.07220500	4.17748500
C	6.92700600	1.96275500	4.69604700
C	6.66352900	4.38302000	4.47732200
C	8.06204000	2.16503300	5.48631100
C	7.79990200	4.57106800	5.26919300
H	6.11073000	5.23984700	4.08252800
C	8.50349100	3.46638900	5.77622300
H	8.60602700	1.30159500	5.88058600
H	9.39154200	3.61903900	6.39621700
C	-4.05836400	2.69926800	-2.66949300
C	-5.05667200	2.87409600	-3.37064400
C	-6.20888800	3.07400500	-4.17705300
C	-6.66245800	4.38488900	-4.47717700
C	-6.92683100	1.96465200	-4.69513400
C	-7.79893600	4.57310300	-5.26886000
H	-6.10927600	5.24164100	-4.08275500
C	-8.06196300	2.16709500	-5.48521300
C	-8.50301900	3.46852200	-5.77541400
H	-8.60633900	1.30373300	-5.87911700
H	-9.39115000	3.62130000	-6.39526200
H	6.57757100	0.95160300	4.46963000
H	8.13899300	5.58665200	5.49392500
H	-6.57770000	0.95344600	-4.46848700
H	-8.13771900	5.58873900	-5.49381800
Zn	0.00000300	-0.00000100	-0.00006100
N	1.16847100	-1.32751100	-0.91378700
C	0.96684300	-2.70279400	-0.70820900
C	2.32030000	-1.18738300	-1.60527400
C	2.03689600	-3.45261000	-1.33586700
N	-0.00074300	-3.27787900	-0.00022000
C	2.90923500	-2.48512700	-1.88412600
C	2.85047600	0.11440600	-2.02388800
C	2.17823800	-4.91023400	-1.37896500
C	-0.96803300	-2.70240100	0.70786200
C	4.05838200	-2.69931400	-2.66944200
C	1.98652200	1.14439100	-2.46160900
C	4.24282900	0.36408400	-1.98875500
C	1.04501300	-5.75675600	-1.45743500
C	3.46187000	-5.50960600	-1.35781600
C	-2.03837000	-3.45177600	1.33554400
N	-1.16899100	-1.32705100	0.91361900
C	5.05662900	-2.87434600	-3.37062800
C	2.49816000	2.38882600	-2.84510700
H	0.91124300	0.95686800	-2.52832500
C	4.74838500	1.61265600	-2.36783900
H	4.91971800	-0.41824500	-1.63823900
C	1.19499600	-7.14675200	-1.51665500
H	0.04856100	-5.31186700	-1.47019300
C	3.60528600	-6.89986700	-1.41634200
H	4.34693600	-4.87412500	-1.27687100
C	-2.91016200	-2.48395100	1.88407100
C	-2.18043800	-4.90934100	1.37841000
C	-2.32064900	-1.18645000	1.60531000
C	6.20880500	-3.07440500	-4.17705900
C	3.88006700	2.62862800	-2.79689800
H	1.81469100	3.17147400	-3.18706900
H	5.82583600	1.79625000	-2.31991500

C	2.47321600	-7.72596600	-1.49865300
H	0.30526200	-7.78062800	-1.57851500
H	4.60630600	-7.34131700	-1.38967700
C	-4.05925900	-2.69777600	2.66956100
C	-1.04763700	-5.75643200	1.45681500
C	-3.46436600	-5.50806700	1.35705400
C	-2.85011600	0.11554600	2.02415900
C	6.66231400	-4.38534800	-4.47702100
C	6.92676400	-1.96515100	-4.69532600
H	4.27866200	3.60301500	-3.09377100
H	2.58681200	-8.81312700	-1.54697300
C	-5.05743600	-2.87255900	3.37090900
C	-1.19831700	-7.14636500	1.51578800
H	-0.05096400	-5.31204300	1.46973200
C	-3.60847900	-6.89826800	1.41532800
H	-4.34910000	-4.87212000	1.27613900
C	-1.98553600	1.14521300	2.46140300
C	-4.24239000	0.36576600	1.98975100
C	7.79875200	-4.57371200	-5.26872500
H	6.10911800	-5.24202400	-4.08245400
C	8.06185700	-2.16774300	-5.48542300
H	6.57767800	-0.95390000	-4.46880900
C	-6.20953600	-3.07239000	4.17750400
C	-2.47682400	-7.72493900	1.49758900
H	-0.30890600	-7.78069700	1.57760900
H	-4.60971700	-7.33921600	1.38850400
C	-2.49649000	2.38984700	2.84515400
H	-0.91028800	0.95729200	2.52752200
C	-4.74726400	1.61453600	2.36909200
H	-4.91976800	-0.41630600	1.63960900
C	8.50285500	-3.46922600	-5.77546100
H	8.13748900	-5.58939200	-5.49355500
H	8.60624700	-1.30445600	-5.87946900
C	-6.92702600	-1.96300800	4.69614900
C	-6.66344200	-4.38324500	4.47724800
H	-2.59096000	-8.81205300	1.54570900
C	-3.87833200	2.63017700	2.79768700
H	-1.81253800	3.17223500	3.18674700
H	-5.82467000	1.79854000	2.32173600
H	9.39095500	-3.62212100	-6.39532400
C	-8.06205400	-2.16539100	5.48639200
H	-6.57763400	-0.95182400	4.46980500
C	-7.79980900	-4.57140000	5.26910300
H	-6.11060700	-5.24002000	4.08239100
H	-4.27639700	3.60471700	3.09477100
C	-8.50344900	-3.46678900	5.77620900
H	-8.60608200	-1.30200700	5.88072800
H	-8.13885500	-5.58701500	5.49376000
H	-9.39149700	-3.61952200	6.39618700

Frequencies (cm⁻¹):

6.8342	8.1829	9.6196
10.4965	10.6331	11.3848
13.5137	15.0126	18.0901
19.8135	19.8173	20.1431
25.9652	26.3413	27.3281
28.1970	28.2465	29.7427
32.1864	41.3647	43.6390
45.9646	48.5286	49.8069
49.9094	53.5961	54.6895
54.9437	56.3507	57.6452
62.8486	63.5737	66.9884

67.7438	71.5712	73.1358
74.1787	74.8729	77.0236
78.5287	99.1123	99.7038
105.9848	109.4982	110.0995
116.5383	117.6125	119.2071
132.4688	138.5386	140.2256
143.4119	145.1979	150.0796
163.0473	187.2347	190.8637
193.9399	194.6712	202.2898
208.5581	208.8833	210.1230
211.8736	215.9805	218.8134
226.5699	226.8917	227.5153
228.0654	229.1294	237.6769
239.4037	264.2168	264.9809
286.5773	289.7034	313.7336
319.3544	333.5456	334.5963
339.2121	340.9819	355.0770
355.1561	361.6007	362.2540
377.4262	377.9179	385.5204
388.2950	395.4379	395.4454
395.4598	395.4656	398.3156
398.3765	399.7929	400.9363
401.5577	402.1114	402.9708
403.0786	419.9413	419.9588
439.8840	442.3491	444.6667
446.1260	468.2033	468.2559
479.1060	483.0723	489.5107
489.8101	497.4083	497.5908
498.2354	498.2904	503.5227
503.5695	504.1740	504.4196
521.9689	522.5200	536.3929
536.4602	543.3229	543.5223
571.9384	572.4961	592.4252
592.4578	596.5928	596.7422
608.4808	608.7764	608.8313
609.3125	609.5297	609.5650
609.6049	609.6647	613.2737
613.2750	613.4302	613.4323
641.4231	642.4352	661.4146
661.4754	664.5833	666.3695
676.1425	676.9991	678.0587
678.1664	679.6361	679.9698
680.4874	680.5115	680.5549
680.6866	680.7817	683.1449
683.4142	684.0954	691.9634
692.1185	696.0443	696.8109
707.3446	708.1309	711.7720
712.5022	719.8958	723.0773
737.9487	738.2835	743.0691
743.0969	743.1410	743.1504
758.4467	758.5279	760.5039
760.6448	760.8165	761.4390
768.2311	768.4585	793.8914
794.0630	809.6604	811.7370
816.1786	816.2389	819.2399
819.7756	820.3004	822.7662
822.8088	824.8296	824.9510
824.9920	825.0435	826.8694
840.3515	841.0618	872.7082
872.8001	891.5937	891.8359
893.1575	893.2547	893.3965

893.4121	893.5232	893.5879
895.8864	897.5636	898.3770
901.0185	930.6606	930.6628
933.2709	933.3063	937.6027
938.0375	938.0414	938.0470
938.0569	938.5058	939.5889
940.8112	954.6951	954.6975
956.0317	956.0421	962.4655
962.5461	962.5476	962.5495
962.5502	962.6735	963.3014
963.6967	977.2752	977.4880
978.3464	979.3221	981.8699
981.8722	981.8823	981.8826
983.1291	983.4960	983.5617
983.8032	984.8614	985.0196
986.1100	986.3868	1019.3938
1020.5891	1025.5746	1025.6149
1026.8178	1027.1159	1027.7343
1028.2244	1033.6310	1033.7902
1033.9808	1034.0157	1040.4262
1041.9969	1059.6405	1060.2634
1076.4685	1076.4703	1076.4730
1076.4751	1080.5543	1081.1418
1083.2307	1084.2004	1085.1724
1085.2854	1091.5696	1091.6969
1149.6751	1149.6754	1149.6775
1149.6779	1149.8379	1149.8437
1149.8692	1149.8768	1151.3449
1151.3894	1151.4716	1151.7618
1153.5634	1154.1789	1159.5059
1159.8121	1164.0370	1164.3835
1168.6900	1170.0281	1170.5293
1170.9622	1171.5459	1172.4843
1172.4880	1173.6529	1174.5063
1174.6860	1174.8921	1174.9816
1183.2375	1184.0702	1253.4420
1253.5978	1254.7515	1255.6820
1278.6541	1280.9944	1291.0900
1291.5811	1291.6531	1291.6554
1292.0420	1295.0023	1299.4860
1299.5621	1304.2842	1304.3041
1316.9213	1317.3905	1334.3245
1340.8718	1349.1224	1349.1230
1349.1343	1349.1439	1355.4392
1355.4430	1355.7689	1355.8348
1360.0935	1360.4757	1360.9036
1362.0974	1381.5728	1382.0002
1389.7159	1389.7826	1419.1132
1419.8578	1426.6451	1426.9645
1435.1854	1436.0060	1436.2850
1436.3037	1437.3879	1437.4577
1437.5054	1437.5201	1440.9377
1441.2431	1442.2860	1443.3527
1466.0269	1466.4238	1469.1094
1469.1169	1474.6415	1475.8826
1493.0410	1493.0725	1495.2279
1495.9235	1496.2781	1496.4161
1502.5227	1504.9580	1523.5161
1523.6541	1524.7548	1525.5152
1560.9660	1562.1733	1570.8591
1570.8595	1570.8601	1570.8603

1577.1814	1577.2570	1577.4087
1577.4391	1580.8814	1581.2235
1581.8682	1581.9877	1605.7358
1606.0288	1606.5326	1606.5510
1606.5955	1606.6524	1606.8262
1607.0787	1607.1003	1607.1145
1608.0577	1608.0604	2223.7425
2223.9800	2224.4009	2224.4245
3116.4888	3116.4893	3116.6990
3116.7026	3120.0161	3120.0165
3120.0215	3120.0257	3121.5785
3121.6194	3121.6970	3121.7017
3125.5151	3125.5187	3126.1658
3126.1688	3126.6875	3126.6877
3126.6895	3126.6898	3128.5074
3128.5719	3128.8174	3128.8721
3136.1972	3136.1978	3136.2013
3136.2045	3137.0301	3137.0756
3137.3493	3137.3844	3138.3626
3138.3632	3138.6521	3138.6774
3142.0124	3142.0134	3142.0143
3142.0178	3145.8020	3145.9066
3145.9358	3145.9368	3147.9260
3147.9279	3147.9528	3147.9691
3149.1984	3149.2045	3149.2493
3149.2562	3154.8536	3154.8713
3155.1687	3155.2264	3163.4925
3163.4985	3164.1310	3164.1372