

Supporting Information Accompanying:

A TDDFT Description of the Low-Energy Excited States of Copper and Zinc Metalloenediynes

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Table 2S. TDDFT Results

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2S2: **2** B3LYP / 6-31G* Rotational Isomer #1
2S3: **3** B3LYP / 6-31G* Rotational Isomer #1
2S4: **4** B3LYP / 6-31G* Rotational Isomer #1

Table 1s. Calculated Structural Parameters (in Å)

1S1: 1 B3LYP / 6-31G*

C1	2.970875	-2.3146	1.163111
C2	2.895334	-1.32025	0.174031
C3	1.811226	-1.33571	-0.7051
C4	0.861036	-2.35076	-0.55924
C5	1.028452	-3.29351	0.452487
N6	2.064816	-3.27967	1.305638
O7	3.919173	-0.41107	0.169768
C8	4.012708	0.506051	-0.91967
C9	3.086937	1.638162	-0.83898
C10	2.335601	2.590465	-0.78103
C11	1.524645	3.750832	-0.76807
C12	0.323346	3.88571	-0.15488
C13	-0.34732	2.88713	0.59198
C14	-0.97401	2.081832	1.249643
C15	-1.73731	1.119804	2.045535
O16	-3.05691	0.877236	1.539614
C17	-3.20066	0.091864	0.430814
C18	-4.51348	-0.16537	0.019476
C19	-4.71663	-0.97878	-1.08798
C20	-3.60524	-1.51227	-1.74696
N21	-2.34931	-1.26645	-1.36503
C22	-2.15013	-0.4751	-0.30218
H23	-0.17778	4.848959	-0.23255
H24	1.919131	4.613724	-1.3022
H25	-1.18991	0.173099	2.147302
H26	-1.90559	1.51549	3.052193
H28	5.044748	0.870391	-0.88483
H29	3.88307	-0.02678	-1.87323
H30	-5.33805	0.270728	0.575111
H31	1.684776	-0.5761	-1.46866
H32	-5.72136	-1.20162	-1.43515
H33	-0.00952	-2.38142	-1.20905
H34	-3.7295	-2.15863	-2.61337
H35	0.302903	-4.09243	0.591023
H36	-1.11359	-0.29056	-0.03832
H37	3.811739	-2.30435	1.854456

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1S2: 2 B3LYP / 6-31G* Rotational Isomer #1

C1	-4.022348	-1.401512	1.114401
C2	-4.567334	-0.781541	0.224041
C3	-5.268960	-0.128025	-0.816463
C4	-4.867559	0.978236	-1.489426
C5	-3.687085	1.734660	-1.286481
C6	-2.721845	2.467349	-1.197939
C7	-1.642016	3.456197	-1.172390
O8	-1.068072	3.680009	0.118378
C9	0.084938	3.027967	0.458765
C10	0.832121	3.592559	1.500185
C11	2.021580	2.981700	1.875613
C12	2.441983	1.829421	1.206922
N13	1.716414	1.279241	0.220717
C14	0.557209	1.858138	-0.143510
Cu15	2.489642	-0.609599	-0.550570
N16	3.578846	-0.544575	-2.421965
Cl17	4.574931	-0.887410	0.613929
N18	0.817550	-1.836631	-0.293022
C19	0.426023	-2.772651	-1.179602
C20	-0.770061	-3.467546	-1.046593
C21	-1.610433	-3.197849	0.035766
C22	-1.194077	-2.242106	0.965088
C23	0.027709	-1.591076	0.759058
O24	-1.870093	-1.872240	2.092459
C25	-3.279082	-2.116580	2.151758
H26	-6.220818	-0.571330	-1.103763
H27	-5.524759	1.346541	-2.275925
H28	-0.857228	3.197190	-1.896015
H29	-2.051091	4.428939	-1.469669
H30	0.468052	4.495071	1.981442
H31	2.628104	3.393713	2.676243
H32	3.365843	1.308431	1.448616
H33	-0.006543	1.351303	-0.920896
H34	0.358064	-0.838880	1.467133
H35	1.096014	-2.951265	-2.014338
H36	-1.051633	-4.208920	-1.788019
H37	-2.556094	-3.718193	0.136500
H38	-3.487114	-3.195369	2.108853
H39	-3.570651	-1.770154	3.148185
H40	4.459716	-0.679346	-1.916161
H41	3.497036	-1.281679	-3.120367
H42	3.630728	0.345856	-2.914026

1S3: 2 B3LYP / 6-31G* Rotational Isomer #2

C1	2.350616	2.856816	0.396761
C2	3.150712	2.443700	-0.417876
C3	4.094008	2.054026	-1.400374
C4	4.736547	0.861482	-1.464853
C5	4.548242	-0.222713	-0.574756
C6	4.415440	-1.184344	0.154313
C7	4.135449	-2.311588	1.043364
O8	2.776111	-2.331993	1.495522
C9	1.785181	-2.455647	0.558060
C10	1.915183	-3.061844	-0.693292
C11	0.783827	-3.137212	-1.508202
C12	-0.422025	-2.595994	-1.074496
N13	-0.536360	-1.992835	0.126699
C14	0.538104	-1.937337	0.922783
Cu15	-2.278660	-0.865715	0.400400
N16	-1.915855	1.184009	0.030459
C17	-2.851106	1.812654	-0.699901
C18	-2.780847	3.182095	-0.962025
C19	-1.716137	3.919225	-0.460288
C20	-0.731511	3.259739	0.285898
C21	-0.867554	1.885176	0.500348
O22	0.278509	4.043629	0.771671
C23	1.421457	3.426788	1.374195
Cl24	-3.881849	-1.529173	-1.334498
N25	-3.710728	-1.423986	1.891621
H26	4.322042	2.793424	-2.166149
H27	5.448355	0.710027	-2.274210
H28	4.724096	-2.238330	1.963400
H29	4.400559	-3.264584	0.564382
H30	2.863051	-3.463462	-1.034570
H31	0.842469	-3.607120	-2.485061
H32	-1.327610	-2.611084	-1.675520
H33	0.424993	-1.459069	1.891605
H34	-0.125170	1.313047	1.045289
H35	-3.645552	1.178145	-1.084283
H36	-3.553938	3.658691	-1.556733
H37	-1.618706	4.986397	-0.634091
H38	1.115430	2.681017	2.119311
H39	1.910308	4.243375	1.915886
H40	-4.143489	-0.711829	2.477017
H41	-3.508474	-2.232684	2.476531
H42	-4.385671	-1.707795	1.175110

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1S4: 3 B3LYP / 6-31G* Rotational Isomer #1

C1	2.700385	2.234061	1.447080
C2	3.740564	1.610673	1.373616
C3	5.013881	0.989191	1.397459
C4	5.456739	-0.027831	0.618659
C5	4.722706	-0.712309	-0.378883
C6	4.162747	-1.356114	-1.242696
C7	3.407334	-2.110873	-2.241162
O8	2.000600	-1.836631	-2.198706
C9	1.322738	-2.110576	-1.048829
C10	1.738493	-2.975289	-0.032157
C11	0.902669	-3.149395	1.070942
C12	-0.299538	-2.454973	1.148927
N13	-0.683258	-1.612022	0.171829
C14	0.098142	-1.451371	-0.902914
Cu15	-2.519715	-0.559781	0.245219
N16	-1.633224	1.235764	-0.535514
C17	-2.217084	1.925115	-1.524475
C18	-1.726511	3.166545	-1.934607
C19	-0.631010	3.713860	-1.284127
C20	-0.036198	3.000995	-0.232300
C21	-0.557761	1.746968	0.096659
O22	1.010681	3.612560	0.383728
C23	1.527991	3.092721	1.617748
Cl24	-4.465863	-0.460917	-0.936835
Cl25	-3.170190	-1.248215	2.329510
H26	5.713173	1.394742	2.127110
H27	6.479609	-.367374	0.771800
H28	3.590106	-3.190059	-2.137631
H29	3.705046	-1.827154	-3.255151
H30	2.687504	-3.496481	-0.084344
H31	1.189933	-3.817028	1.876713
H32	-0.981961	-2.541745	1.987644
H33	-0.236328	-0.765912	-1.673882
H34	-0.117178	1.122727	0.865585
H35	-3.095109	1.464089	-1.964550
H36	-0.224488	4.683150	-1.555201
H38	0.735587	2.589332	2.185458
H39	1.819402	3.981463	2.187979

1S5: **3** B3LYP / 6-31G* Rotational Isomer #2

C1	2.458974	2.605585	0.817920
C2	3.485342	2.328174	0.230893
C3	4.709082	2.123385	-0.453719
C4	5.358953	0.943829	-0.611584
C5	4.906387	-0.318446	-0.159154
C6	4.560943	-1.429082	0.189268
C7	4.022737	-2.733762	0.572879
O8	2.619321	-2.692202	0.864178
C9	1.764025	-2.288224	-0.113543
C10	2.063251	-2.186759	-1.474923
C11	1.065025	-1.743750	-2.344387
C12	-0.180543	-1.398197	-1.838154
N13	-0.460905	-1.506453	-0.525087
C14	0.473526	-1.952926	0.319070
Cu15	-2.372267	-0.923632	0.118158
N16	-1.995088	1.150689	-0.329246
C17	-2.936426	1.921152	-0.888991
C18	-2.799189	3.309533	-0.949766
C19	-1.683189	3.908355	-0.384516
C20	-0.709693	3.100723	0.221994
C21	-0.891881	1.715415	0.199850
O22	0.332978	3.757424	0.799012
C23	1.292943	3.037841	1.589105
Cl24	-2.337783	-2.057938	2.107391
Cl25	-4.511561	-1.025014	-0.647316
H26	5.173156	3.013211	-0.875689
H27	6.307404	0.953787	-1.145500
H28	4.478207	-3.091600	1.500930
H29	4.228143	-3.484535	-0.203857
H30	3.046486	-2.431297	-1.859075
H31	1.260936	-1.656638	-3.408076
H32	-0.974739	-1.024314	-2.475876
H33	0.183653	-2.055620	1.360435
H34	-0.155695	1.031804	0.606004
H35	-3.809975	1.398730	-1.264716
H36	-3.573003	3.908107	-1.419286
H37	-1.544535	4.984969	-0.384943
H38	0.814592	2.201900	2.113230
H39	1.611903	3.758511	2.349916

1S6: 4 B3LYP / 6-31G* Rotational Isomer #1

C1	2.671195	2.448466	1.110412
C2	4.036737	-1.583629	-1.113862
C3	3.702626	1.810927	1.033671
C4	4.611791	-0.777361	-0.411005
C5	4.983849	1.205209	1.042414
C6	5.388935	0.081018	0.403061
C7	1.514272	3.333927	1.253334
C8	3.296915	-2.549327	-1.925713
O9	0.934834	3.718280	-0.002902
O10	1.881086	-2.327186	-1.920702
C11	-0.076783	2.991121	-0.546167
C12	1.220642	-2.382794	-0.731242
C13	-0.589968	3.471389	-1.760857
C14	1.693661	-2.966465	0.447813
C15	-1.647218	2.804581	-2.362087
C16	0.882989	-2.923446	1.582620
C17	-2.177047	1.670472	-1.744262
C18	-0.351321	-2.286994	1.525009
N19	-1.678608	1.210038	-0.588378
N20	-0.799646	-1.730893	0.383411
C21	-0.649536	1.842930	0.006398
C22	-0.045505	-1.788041	-0.719112
Zn23	-2.601384	-0.512162	0.385383
Cl24	-4.109998	-1.234834	-1.195576
Cl25	-2.756364	0.004297	2.634705
H26	5.732823	1.727789	1.635837
H27	6.430274	-0.211761	0.527191
H28	0.754985	2.909369	1.920783
H29	1.841657	4.279102	1.698682
H30	3.522319	-3.577481	-1.607443
H31	3.576410	-2.467634	-2.980473
H32	-0.149115	4.361848	-2.197945
H33	2.671974	-3.430519	0.496136
H34	-2.066258	3.157205	-3.298739
H35	1.220220	-3.364171	2.514978
H36	-3.006560	1.106437	-2.160278
H37	-0.993994	-2.175191	2.391948
H38	-0.307201	1.408157	0.938279
H39	-0.434838	-1.333817	-1.624593

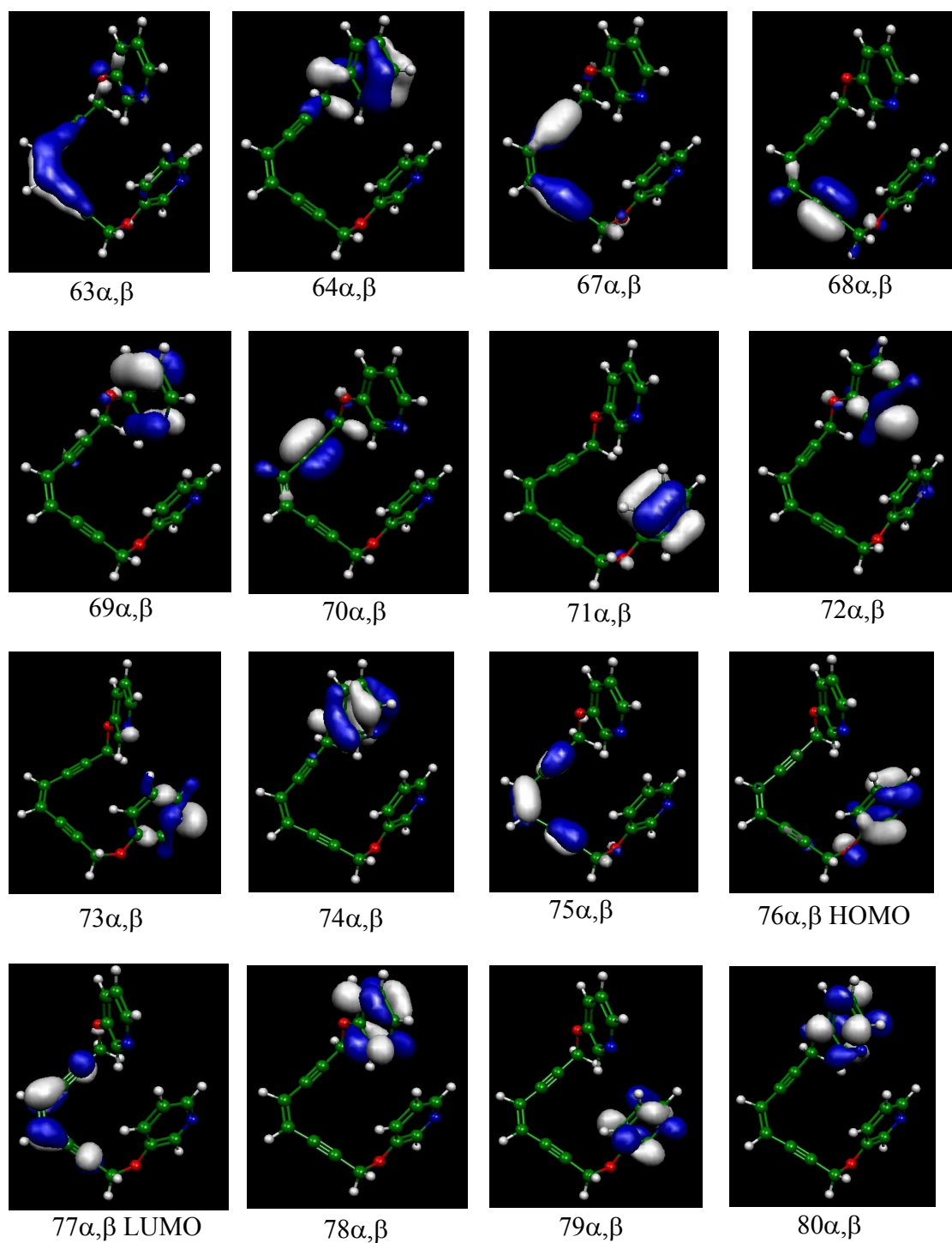
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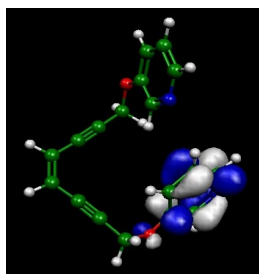
1S7: 4 B3LYP / 6-31G* Rotational Isomer #2

C1	2.389828	2.776789	0.597939
C2	3.295513	2.406586	-0.121459
C3	4.364935	2.088997	-0.995319
C4	4.975563	0.885181	-1.124328
C5	4.636705	-0.297287	-0.424236
C6	4.394309	-1.343621	0.141761
C7	3.991977	-2.568527	0.831250
O8	2.605464	-2.560708	1.196935
C9	1.672007	-2.490839	0.207155
C10	1.859901	-2.860548	-1.127485
C11	-0.439752	-2.277369	-1.544328
N13	-0.601439	-1.897163	-0.262693
C14	0.416802	-2.010082	0.597827
Zn15	-2.396405	-0.848503	0.356394
N16	-1.917132	1.182808	-0.281181
C17	-2.630048	1.786760	-1.242992
C18	-2.394539	3.116236	-1.593903
C19	-1.395349	3.823782	-0.938387
C20	-0.649569	3.186472	0.062674
C21	-0.947713	1.855563	0.364697
O22	0.284943	3.947786	0.697536
C23	1.329468	3.311517	1.453944
Cl24	-2.096675	-0.70567	2.649728
Cl25	-4.023179	-1.495727	-1.146990
H26	4.731313	2.906051	-1.614679
H27	5.796647	0.807161	-1.834692
H28	4.519245	-2.672586	1.784450
H29	4.228615	-3.457149	0.229466
H30	2.819240	-3.216358	-1.486324
H31	0.886429	-3.055189	-3.044217
H32	-1.311711	-2.179338	-2.183598
H33	0.233298	-1.706036	1.624510
H34	-0.442988	1.306187	1.150728
H35	-3.397514	1.180972	-1.715349
H36	-2.989786	3.585451	-2.370354
H37	-1.175940	4.860225	-1.174989
H38	0.922924	2.548324	2.127120
H39	1.727718	4.115333	2.081038

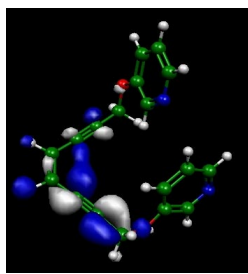
Figure 1S. UB3LYP Molecular Orbitals of **1**



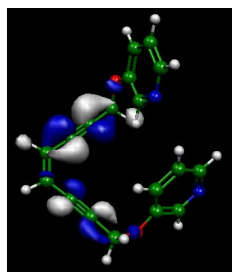
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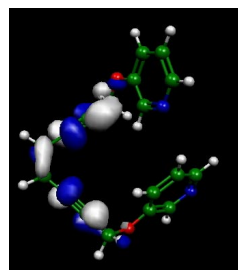
81 α,β



82 α,β



83 α,β



84 α,β

Figure 2S. UB3LYP Molecular Orbitals of **2**

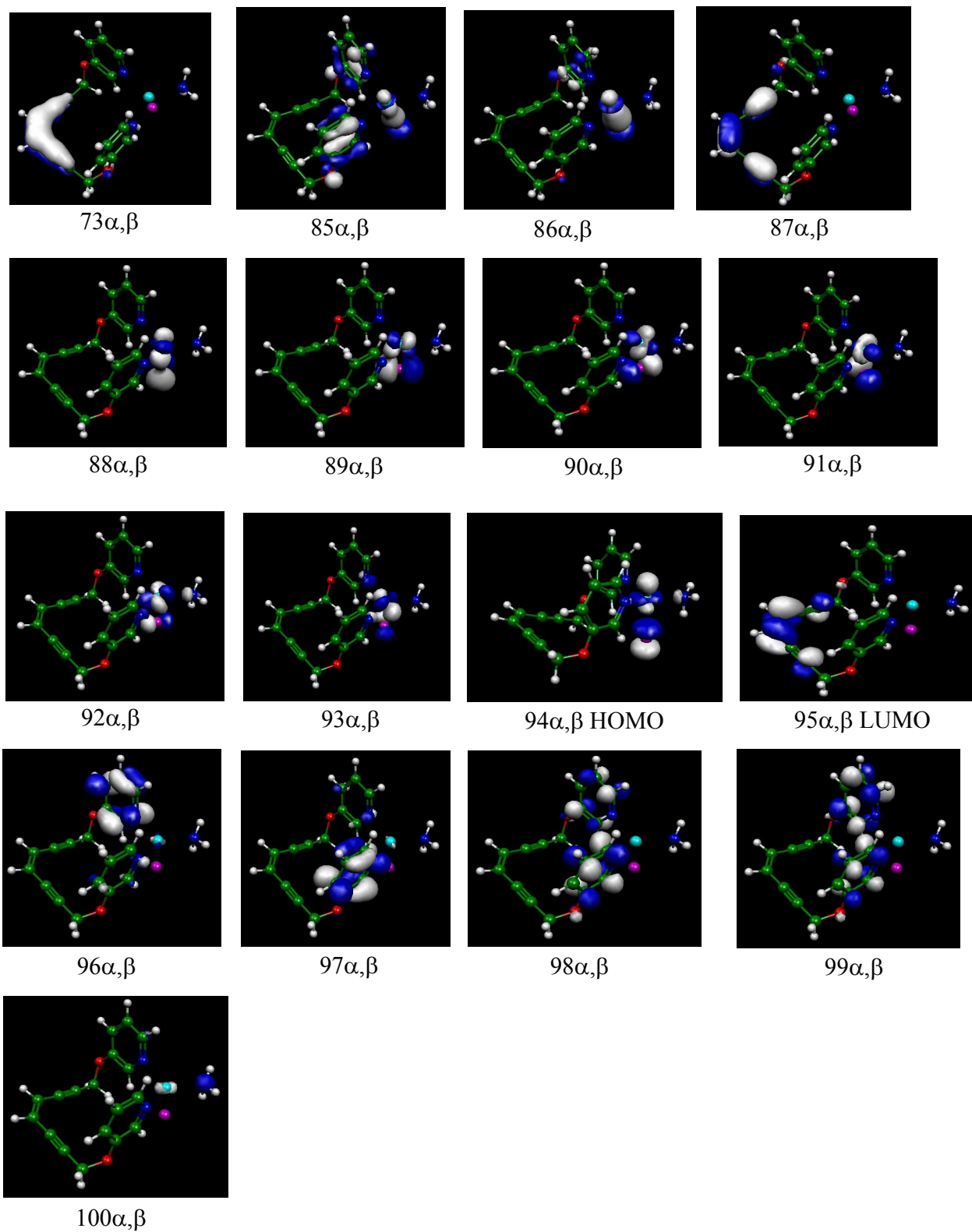
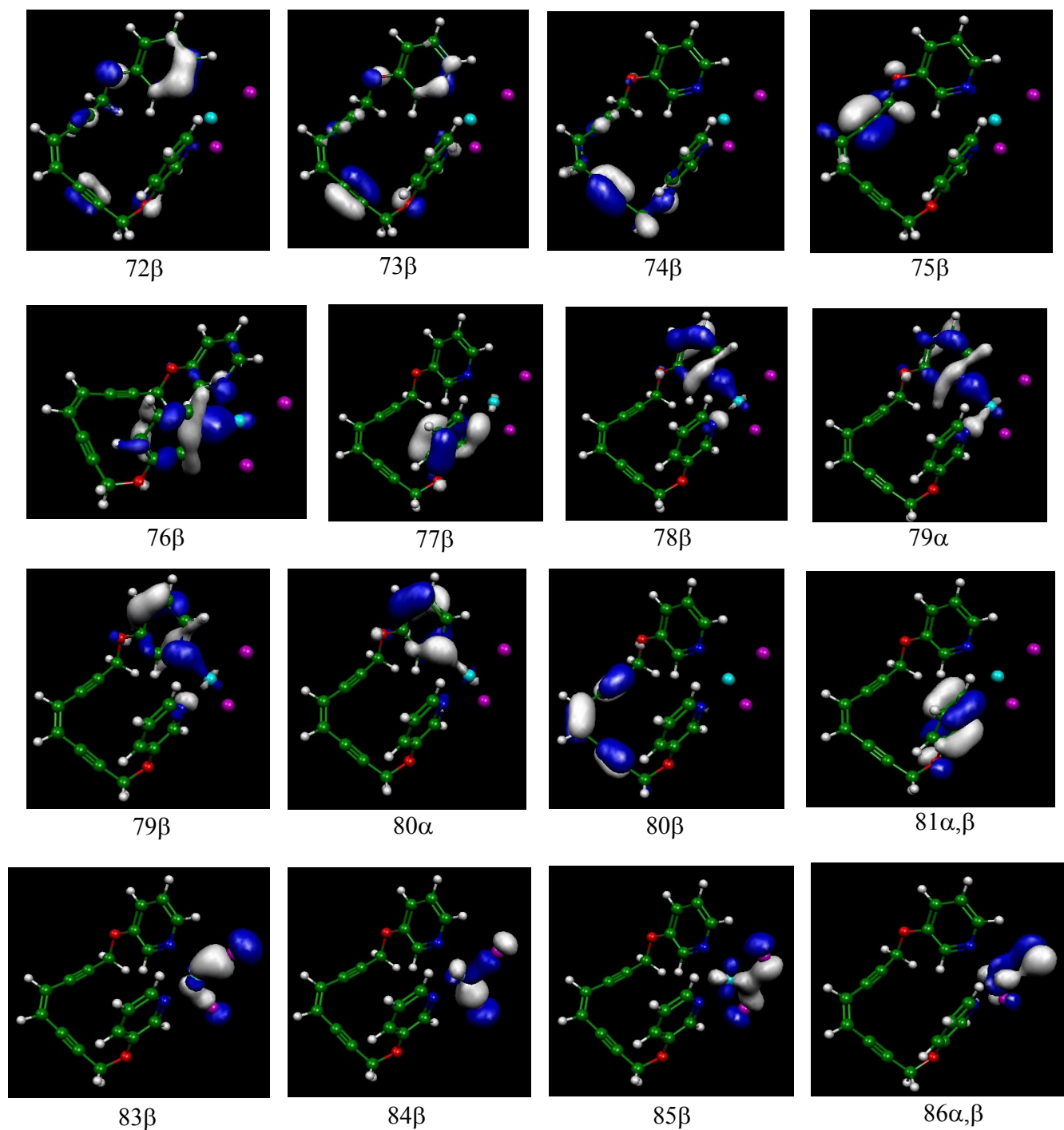
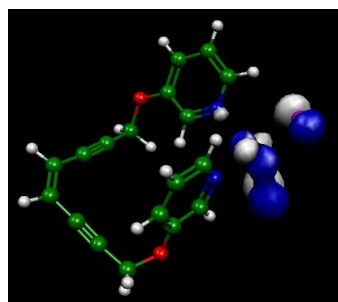
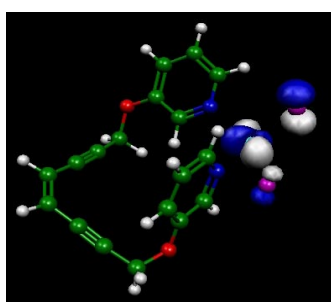


Figure 3S. UB3LYP Molecular Orbitals of **3**

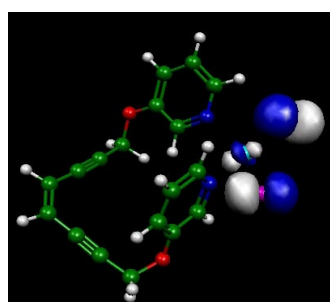




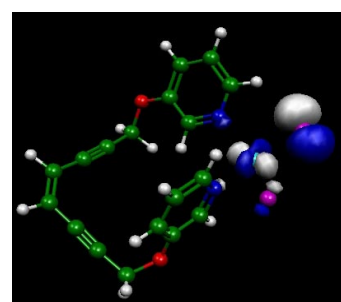
87 α,β



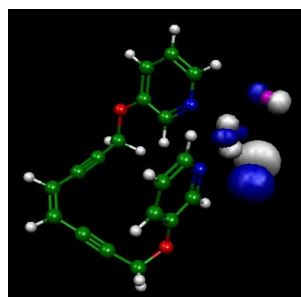
88 β



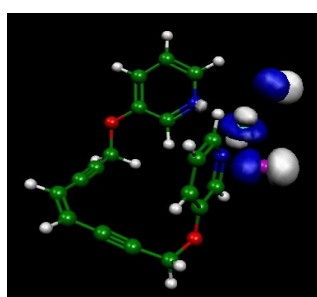
89 α,β



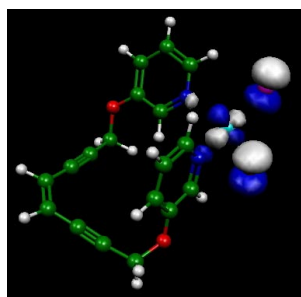
90 α,β



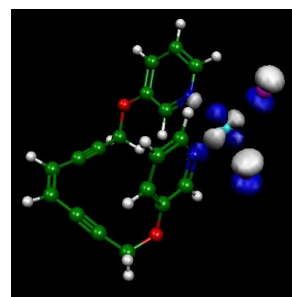
91 α,β



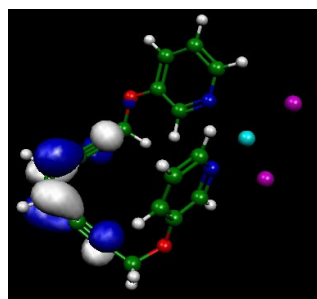
92 α,β



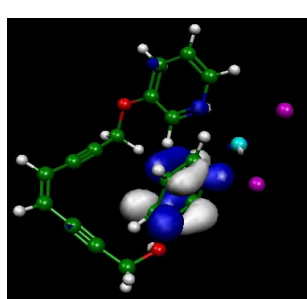
93 α HOMO



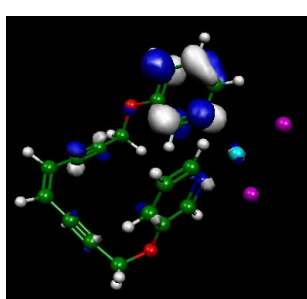
93 β LUMO



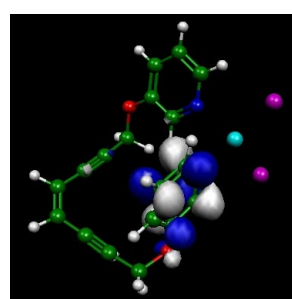
94 α,β



95 α,β

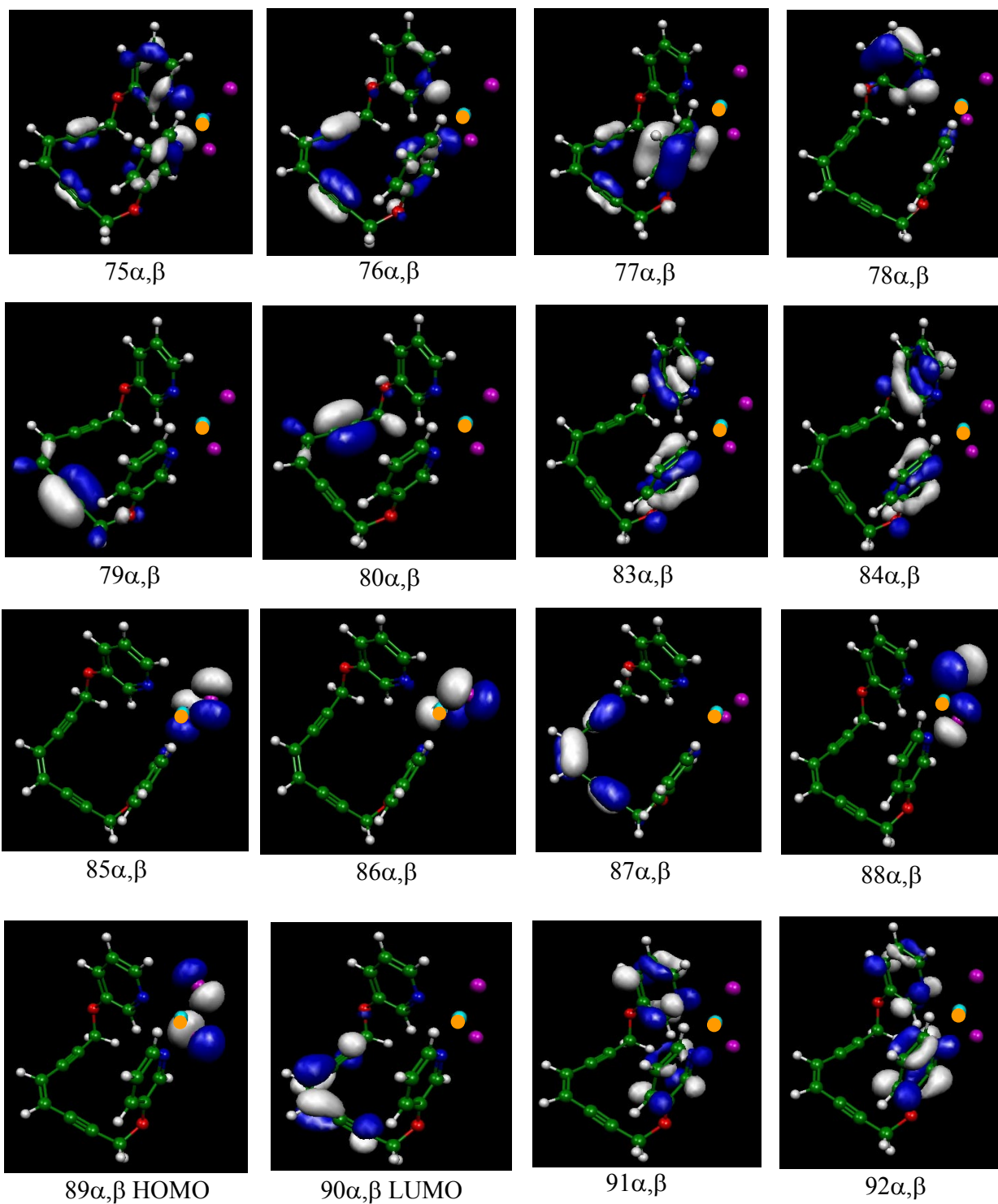


96 α,β

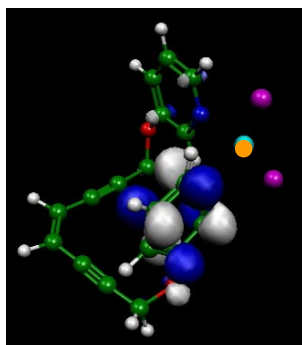


97 α,β

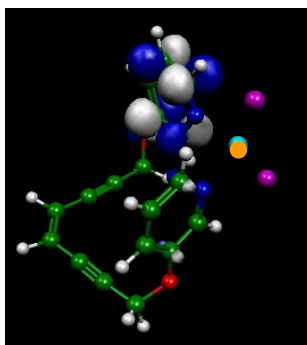
Figure 4S. UB3LYP Molecular Orbitals of 4



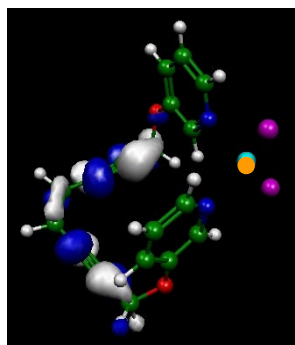
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93 α,β



94 α,β



98 α,β

Table 2S. TDDFT Results

2S1: 1 UB3LYP / 6-31G*

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Triplet	2.3583	525.73	63A -> 77A	-.10179
				67A -> 84A	.12181
				74A -> 77A	.17316
				75A -> 77A	.76156
				76A -> 77A	-.30037
				63B -> 77B	.10179
				67B -> 84B	-.12181
				74B -> 77B	-.17316
				75B -> 77B	-.76156
				76B -> 77B	.30037
2	Triplet	3.7786	328.12	71A -> 79A	.36208
				75A -> 77A	.13383
				75A -> 81A	.15390
				76A -> 77A	.34124
				76A -> 79A	.13731
				76A -> 81A	.52509
				71B -> 79B	-.36208
				75B -> 77B	-.13383
				75B -> 81B	-.15390
				76B -> 77B	-.34124
				76B -> 79B	-.13731
				76B -> 81B	-.52509
3	Triplet	3.7947	326.73	64A -> 78A	.11494
				69A -> 78A	.38473
				70A -> 78A	-.10280
				74A -> 78A	-.40659
				74A -> 79A	-.12424
				74A -> 80A	.48558
				75A -> 80A	-.14073
				64B -> 78B	-.11494
				69B -> 78B	-.38473
				70B -> 78B	.10280
				74B -> 78B	.40659
				74B -> 79B	.12424
				74B -> 80B	-.48558
				75B -> 80B	.14073
4	Singlet	3.8811	319.46	75A -> 77A	.15468
				76A -> 77A	.68601
				75B -> 77B	.15468
				76B -> 77B	.68601
5	Triplet	3.8826	319.33	71A -> 79A	-.23033
				75A -> 77A	.21759
				76A -> 77A	.53170
				76A -> 79A	.12194
				76A -> 81A	-.34658

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				71B -> 79B	.23033
				75B -> 77B	-.21759
				76B -> 77B	-.53170
				76B -> 79B	-.12194
				76B -> 81B	.34658
6	Triplet	3.9530	313.64	69A -> 78A	.18495
				70A -> 77A	-.14760
				74A -> 77A	.51856
				74A -> 78A	.31729
				74A -> 80A	.25942
				75A -> 78A	-.11216
				69B -> 78A	.18495
				70B -> 77B	.14760
				74B -> 77B	-.51856
				74B -> 78B	-.31729
				74B -> 80B	-.25942
				75B -> 78B	.11216
7	Triplet	4.0224	308.23	75A -> 79A	.17817
				76A -> 77A	-.16549
				76A -> 79A	.67393
				75B -> 79B	-.17817
				76B -> 77B	.16549
				76B -> 79B	-.67393
8	Singlet	4.0657	304.95	74A -> 77A	.67116
				75A -> 77A	-.18581
				74B -> 77B	.67116
				75B -> 77B	-.18581
9	Triplet	4.0818	303.75	69A -> 78A	.15743
				70A -> 77A	.22161
				74A -> 77A	-.36043
				74A -> 78A	.48493
				74A -> 80A	.22294
				75A -> 78A	-.14626
				69B -> 78B	-.15743
				70B -> 77B	-.22161
				74B -> 77B	.36043
				74B -> 78B	-.48493
				74B -> 80B	-.22294
				75B -> 78B	.14626
10	Triplet	4.1527	298.56	72A -> 79A	-.13206
				73A -> 77A	.14528
				73A -> 79A	.67551
				73A -> 80A	.10106
				73A -> 81A	-.10975
				72B -> 79B	.13206
				73B -> 77B	-.14528
				73B -> 79B	-.67551
				73B -> 80B	-.10106
				73B -> 81B	.10975
11	Triplet	4.2065	294.74	72A -> 77A	-.14912
				72A -> 78A	-.66053
				73A -> 78A	-.20344
				72B -> 77B	.14912
				72B -> 78B	.66053

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				73B -> 78B	.20344
12	Triplet	4.2768	289.90	69A -> 77A	-.10486
				70A -> 77A	-.62670
				74A -> 77A	-.25544
				69B -> 77B	.10486
				70B -> 77B	.62670
				74B -> 77B	.25544
13	Triplet	4.3347	286.02	68A -> 77A	.46248
				71A -> 77A	.12160
				73A -> 77A	.48209
				73A -> 79A	-.12626
				68B -> 77B	-.46248
				71B -> 77B	-.12160
				73B -> 77B	-.48209
				73B -> 79B	.12626
14	Singlet	4.4095	281.17	68A -> 77A	.18928
				70A -> 77A	.16694
				73A -> 77A	.51798
				74A -> 77A	.12208
				75A -> 77A	.31431
				68B -> 77B	.18928
				70B -> 77B	.16694
				73B -> 77B	.51798
				74B -> 77B	.12208
				75B -> 77B	.31431
15	Singlet	4.4189	280.57	70A -> 77A	.17845
				73A -> 77A	-.44336
				74A -> 77A	.14957
				75A -> 77A	.41714
				70B -> 77B	.17845
				73B -> 77B	-.44336
				74B -> 77B	.14957
				75B -> 77B	.41714
16	Triplet	4.4209	280.45	67A -> 77A	-.63775
				68A -> 82A	-.16173
				69A -> 77A	-.10729
				70A -> 83A	.14327
				75A -> 84A	-.23147
				67B -> 77B	.63775
				68B -> 82B	.16173
				69B -> 77B	.10729
				70B -> 83B	-.14327
				75B -> 84B	.23147
17	Singlet	4.5474	272.65	69A -> 77A	.11300
				70A -> 77A	.58916
				72A -> 77A	.25368
				75A -> 77A	-.20485
				69B -> 77B	.11300
				70B -> 77B	.58916
				72B -> 77B	.25368
				75B -> 77B	-.20485
18	Triplet	4.5607	271.85	68A -> 77A	-.45561
				71A -> 77A	-.12663
				72A -> 77A	.12582

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				73A -> 77A	.47802
				75A -> 82A	-.10877
				68A -> 77A	-.45561
				71B -> 77B	.12663
				72B -> 77B	-.12582
				73B -> 77B	-.47802
				75B -> 82B	.10877
19	Singlet	4.7152	262.94	68A -> 77A	-.16660
				70A -> 77A	-.21181
				72A -> 77A	.61432
				72A -> 78A	.12366
				75A -> 77A	.10432
				68B -> 77B	-.16660
				70B -> 77B	-.21181
				72B -> 77B	.61432
				72B -> 78B	.12366
				75B -> 77B	.10432
20	Triplet	4.7391	261.62	68A -> 77A	.10455
				69A -> 78A	-.10834
				72A -> 77A	.64962
				72A -> 78A	-.11584
				68B -> 77B	-.10455
				69B -> 78B	.10834
				72B -> 77B	-.64962
				72B -> 78B	.11584

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2S2: 2 UB3LYP / 6-31G* Rotational Isomer #1

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Triplet	2.3354	530.88	87A -> 95A	-.33661
				94A -> 95A	-.62601
				94A -> 96A	.12135
				87B -> 95B	.33661
				94B -> 95B	.62601
				94B -> 96B	-.12135
2	Triplet	2.3428	529.22	73A -> 95A	-.10097
				85A -> 95A	.11345
				86A -> 95A	-.12559
				87A -> 95A	.73397
				94A -> 95A	-.28853
				73B -> 95B	.10097
				85B -> 95B	-.11345
				86B -> 95B	.12559
				87B -> 95B	-.73397
				94B -> 95B	.28853
3	Singlet	2.3482	528.00	94A -> 95A	.69918
				94B -> 95B	.69918
4	Triplet	2.5462	486.93	93A -> 95A	.64946
				93A -> 96A	-.23317
				93B -> 95B	-.64946
				93B -> 96B	.23317
5	Singlet	2.5740	481.67	93A -> 95A	.69363
				93A -> 96A	-.12165
				93B -> 95B	.69363
				93B -> 96B	-.12165
6	Triplet	2.7152	456.62	93A -> 95A	.16019
				93A -> 96A	.10300
				93A -> 97A	-.16259
				94A -> 95A	.14352
				94A -> 96A	.53689
				94A -> 97A	-.33153
				93B -> 95B	-.16019
				93B -> 96B	-.10300
				93B -> 97B	.16259
				94B -> 95B	-.14352
				94B -> 96B	-.53689
				94B -> 97B	.33153
7	Triplet	2.7332	453.63	92A -> 95A	.63875
				92A -> 96A	-.23949
				94A -> 96A	.10290
				92B -> 95B	-.63875
				92B -> 96B	.23949
				94B -> 96B	-.10290
8	Singlet	2.7691	447.74	92A -> 95A	.67819
				94A -> 96A	.11528
				92B -> 95B	.67819
				94B -> 96B	.11528

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9	Triplet	2.8011	442.63	93A -> 95A	-.15113
				93A -> 96A	-.31707
				94A -> 96A	.39574
				94A -> 97A	.44687
				93B -> 95B	.15113
				93B -> 96B	.31707
				94B -> 96B	-.39574
				94B -> 97B	-.44687
10	Singlet	2.8041	442.16	92A -> 95A	-.12282
				94A -> 96A	.68347
				92B -> 95B	-.12282
				94B -> 96B	.68347
11	Triplet	2.8419	436.27	93A -> 95A	.13376
				93A -> 96A	.53097
				93A -> 97A	.25178
				94A -> 96A	.13001
				94A -> 97A	.31210
				93B -> 95B	-.13376
				93B -> 96B	-.53097
				93B -> 97B	-.25178
				94B -> 96B	-.13001
				94B -> 97B	-.31210
12	Singlet	2.8744	431.33	94A -> 97A	.68683
				94B -> 97B	.68683
13	Triplet	2.9361	422.28	91A -> 95A	-.31131
				91A -> 97A	-.12430
				93A -> 97A	0.54011
				94A -> 97A	-.26774
				91B -> 95B	.31131
				91B -> 97B	.12430
				93B -> 97B	-0.54011
				94B -> 97B	.26774
14	Singlet	2.9491	420.41	91A -> 95A	.32867
				91A -> 96A	-.11154
				93A -> 95A	.11141
				93A -> 96A	.58165
				91B -> 95B	.32867
				91B -> 96B	-.11154
				93B -> 95B	.11141
				93B -> 96B	.58165
15	Triplet	2.9665	417.94	90A -> 95A	.39667
				90A -> 96A	-.19915
				91A -> 95A	-.34418
				92A -> 95A	-.19482
				92A -> 96A	-.31395
				93A -> 96A	.10603
				93A -> 97A	-.14470
				90B -> 95B	-.39667
				90B -> 96B	.19915
				91B -> 95B	.34418
				92B -> 95B	.19482
				92B -> 96B	.31395

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				93B -> 96B	-.10603
				93B -> 97B	.14470
16	Singlet	2.9812	415.89	91A -> 95A	.61495
				93A -> 96A	-.32256
				91B -> 95B	.61495
				93B -> 96B	-.32256
17	Triplet	2.9850	415.35	90A -> 95A	.29282
				90A -> 96A	-.13214
				91A -> 95A	.50613
				92A -> 95A	-.10150
				92A -> 96A	-.20125
				93A -> 96A	-.12327
				93A -> 97A	.24752
				90B -> 95A	.29282
				90B -> 96A	-.13214
				91B -> 95B	-.50613
				92B -> 95B	.10150
				92B -> 96B	.20125
				93B -> 96B	.12327
				93B -> 97B	-.24752
18	Singlet	3.0175	410.88	90A -> 95A	.62718
				93A -> 97A	-.28669
				90B -> 95B	.62718
				93B -> 97B	-.28669
19	Triplet	3.0570	405.57	90A -> 95A	.48469
				92A -> 95A	.15099
				92A -> 96A	.46480
				90B -> 95B	-.48469
				92B -> 95B	-.15099
				92B -> 96B	-.46480
20	Singlet	3.0692	403.96	90A -> 95A	.29837
				92A -> 96A	.25952
				92A -> 97A	-.10199
				93A -> 97A	.54557
				90B -> 95B	.29837
				92B -> 96B	.25952
				92B -> 97B	-.10199
				93B -> 97B	.54557

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2S3: 3 UB3LYP / 6-31G* Rotational Isomer #1

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Doublet	0.7211	1719.40	73B -> 93B	-.28659
				75B -> 93B	-.11160
				76B -> 93B	-.17682
				78B -> 93B	-.14431
				85B -> 93B	-.25830
				87B -> 93B	-.11054
				90B -> 93B	.69306
				91B -> 93B	.12590
				92B -> 93B	.59306
2	Doublet	0.9455	1311.35	73B -> 93B	-.12025
				75B -> 93B	.29042
				77B -> 93B	-.20485
				78B -> 93B	.11415
				84B -> 93B	.20509
				89B -> 93B	-.49006
				90B -> 93B	.13727
				91B -> 93B	.69160
				92B -> 93B	-.26149
3	Doublet	0.9615	1289.48	73B -> 93B	-.25567
				74B -> 93B	.22748
				77B -> 93B	.17231
				78B -> 93B	.15521
				89B -> 93B	.10414
				90B -> 93B	.65131
				91B -> 93B	-.23188
				92B -> 93B	-.60621
4	Doublet	1.4669	845.18	75B -> 93B	-.10597
				84B -> 93B	-.32820
				89B -> 93B	.68758
				91B -> 93B	.60001
5	Doublet	1.5601	794.71	73B -> 93B	-.19432
				76B -> 93B	.52347
				77B -> 93B	-.27207
				78B -> 93B	-.26779
				79B -> 93B	.21027
				80B -> 93B	.15657
				81B -> 93B	-.23651
				85B -> 93B	.50054
				86B -> 93B	-.17142
				87B -> 93B	.31371
				90B -> 93B	.14233
				92B -> 93B	.10535
6	Doublet	2.0786	596.46	74B -> 93B	-.10900
				75B -> 93B	.37451
				76B -> 93B	-.12844
				77B -> 93B	-.29877
				78B -> 93B	.21376
				79B -> 93B	-.11314

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				80B -> 93B	-.11154
				84B -> 93B	.59716
				85B -> 93B	.12992
				89B -> 93B	.49180
				91B -> 93B	-.15034
7	Doublet	2.2370	554.25	72B -> 93B	-.10049
				73B -> 93B	-.13842
				74B -> 93B	.35776
				75B -> 93B	.20851
				76B -> 93B	.18310
				77B -> 93B	.29120
				78B -> 93B	.58180
				79B -> 93B	-.21726
				81B -> 93B	.17865
				86B -> 93B	.10247
				87B -> 93B	.26734
				92B -> 93B	.37900
8	Quartet	2.3490	527.82	89A -> 94A	-.82180
				89A -> 95A	-.10946
				88B -> 94B	.82530
				88B -> 95B	.10120
9	Doublet	2.5593	484.45	73B -> 93B	-.11319
				78B -> 93B	-.13501
				85B -> 93B	-.30883
				86B -> 93B	.26678
				87B -> 93B	.64312
				88B -> 93B	-.58553
10	Doublet	2.5750	481.49	73B -> 93B	-.26625
				84B -> 93B	.10184
				85B -> 93B	-.41448
				86B -> 93B	-.14338
				87B -> 93B	.40561
				88B -> 93B	.72308
				90B -> 93B	-.13271
11	Doublet	2.6073	475.52	68B -> 93B	-.13305
				73B -> 93B	-.71633
				74B -> 93B	.27203
				76B -> 93B	.11807
				79B -> 93B	.10484
				80B -> 93B	.18047
				81B -> 93B	-.15725
				85B -> 93B	-.12057
				86B -> 93B	.17839
				87B -> 93B	-.43628
				88B -> 93B	-.14842
				90B -> 93B	-.27874
12	Doublet	2.6507	467.74	85B -> 93B	.23117
				86B -> 93B	.90143
				88B -> 93B	.32646
13	Doublet	3.2576	380.59	74B -> 93B	.17080
				75B -> 93B	-.44302
				76B -> 93B	.15722
				77B -> 93B	.38688

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				78B -> 93B	-.14476
				80B -> 93B	.17006
				81B -> 93B	.14661
				84B -> 93B	.60609
				91B -> 93B	.13338
14	Doublet	3.3141	374.11	73B -> 93B	.40485
				75B -> 93B	.14988
				76B -> 93B	.62142
				77B -> 93B	-.12309
				78B -> 93B	.12463
				80B -> 93B	.11621
				81B -> 93B	-.15448
				85B -> 93B	-.46335
				87B -> 93B	-.14520
				90B -> 93B	.13925
15	Quartet	3.6164	342.83	81A -> 96A	-.16816
				86A -> 96A	.12076
				87A -> 95A	.24275
				87A -> 96A	.59120
				87A -> 98A	-.21102
				90A -> 96A	-.19270
				81B -> 96B	.16702
				86B -> 96B	-.18698
				87B -> 95B	-.25171
				87B -> 96B	-.55655
				87B -> 98B	.20290
				89B -> 96B	.14396
16	Doublet	3.6496	339.72	80A -> 95A	-.10191
				86A -> 94A	-.21882
				86A -> 95A	.57068
				86A -> 97A	-.20570
				87A -> 95A	-.12902
				80B -> 95B	.10130
				85B -> 95B	-.14301
				86B -> 94B	.20463
				86B -> 95B	-.52427
				86B -> 96B	.21668
				86B -> 97B	.19717
				87B -> 95B	.17941
				92B -> 94B	.30621
17	Doublet	3.6793	336.98	86A -> 95A	-.17340
				86A -> 97A	.14366
				86B -> 95B	.16504
				86B -> 97B	-.13667
				91B -> 94B	-.12133
				92B -> 94B	.91022
				92B -> 95B	-.10792
18	Doublet	3.6886	336.13	83B -> 93B	.99193
19	Doublet	3.7165	333.60	90B -> 94B	.20114
				91B -> 94B	.91926
				91B -> 95B	-.17769
				91B -> 96B	.11921
				92B -> 94B	.17015

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20	Doublet	3.7979	326.45	79A -> 95A	.11538
				80A -> 95A	.23126
				86A -> 94A	-.13069
				86A -> 95A	.13597
				86A -> 97A	.42455
				91A -> 94A	.11199
				92A -> 94A	-.18094
				93A -> 94A	.53727
				93A -> 95A	-.11997
				80B -> 95B	-.23595
				80B -> 96B	.11089
				85B -> 95B	-.10701
				85B -> 97B	-.14395
				86B -> 94B	.10577
				86B -> 95B	-.11596
				86B -> 97B	-.39491
				87B -> 97B	.11666
				91B -> 94B	.16916
				92B -> 94B	-.10307

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2S4: 4 UB3LYP / 6-31G* Rotational Isomer #1

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Triplet	2.3468	528.30	85A -> 90A	.12715
				87A -> 90A	-.80410
				87A -> 91A	-.15793
				85B -> 90B	-.12715
				87B -> 90B	.80410
				87B -> 91B	.15793
2	Triplet	3.6336	341.22	78A -> 92A	-.10894
				83A -> 92A	-.16239
				84A -> 90A	.14824
				84A -> 91A	-.45840
				84A -> 92A	.44241
				84A -> 94A	.19197
				78B -> 92B	.10894
				83B -> 92B	.16239
				84B -> 90B	-.14824
				84B -> 91B	.45840
				84B -> 92B	-.44241
				84B -> 94B	-.19197
3	Triplet	3.6493	339.74	83A -> 90A	-.24052
				83A -> 91A	.48117
				83A -> 92A	.42720
				83A -> 93A	-.18650
				84A -> 92A	.15716
				83B -> 90B	.24052
				83B -> 91B	-.48117
				83B -> 92B	-.42720
				83B -> 93B	.18650
				84B -> 92B	-.15716
4	Triplet	3.8229	324.32	77A -> 90A	.10411
				77A -> 91A	-.25995
				77A -> 92A	-.24067
				77A -> 93A	-.11289
				83A -> 90A	.14465
				83A -> 91A	-.13527
				83A -> 93A	-.57637
				83A -> 94A	.13837
				84A -> 93A	-.14830
				77B -> 90B	-.10411
				77B -> 91B	.25995
				77B -> 92B	.24067
				77B -> 93B	.11289
				83B -> 90B	-.14465
				83B -> 91B	.13527
				83B -> 93B	.57637
				83B -> 94B	-.13837
				84B -> 93B	.14830
5	Triplet	3.8742	320.02	78A -> 91A	-.24931
				78A -> 92A	.28748

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				78A -> 94A	-.14080
				83A -> 94A	.11234
				84A -> 90A	.16826
				84A -> 92A	.15229
				84A -> 93A	-.11269
				84A -> 94A	-.50242
				86A -> 94A	-.10883
				89A -> 90A	.11035
				78B -> 91B	.24931
				78B -> 92B	-.28748
				78B -> 94B	.14080
				83B -> 94B	-.11234
				84B -> 90B	-.16826
				84B -> 92B	-.15229
				84B -> 93B	.11269
				84B -> 94B	.50242
				86B -> 94B	.10883
				89B -> 90B	-.11035
6	Singlet	4.0589	305.46	86A -> 90A	.11198
				89A -> 90A	.67790
				89A -> 91A	-.10979
				86B -> 90B	.11198
				89B -> 90B	.67790
				89B -> 91B	-.10979
7	Triplet	4.0630	305.15	80A -> 90A	-.19527
				84A -> 90A	-.13908
				84A -> 91A	-.10631
				84A -> 94A	-.11845
				86A -> 90A	-.10960
				89A -> 90A	-.60577
				80B -> 90B	.19527
				84B -> 90B	.13908
				84B -> 91B	.10631
				84B -> 94B	.11845
				86B -> 90B	.10960
				89B -> 90B	.60577
8	Triplet	4.0894	303.19	86A -> 90A	-.10474
				88A -> 90A	-.66909
				88A -> 91A	.12382
				86B -> 90B	.10474
				88B -> 90B	.66909
				88B -> 91B	-.12382
9	Singlet	4.0910	303.06	85A -> 90A	-.10359
				86A -> 90A	.10728
				88A -> 90A	.67739
				88A -> 91A	-.12043
				85B -> 90B	-.10359
				86B -> 90B	.10728
				88B -> 90B	.67739
				88B -> 91B	-.12043
10	Triplet	4.1057	301.98	80A -> 90A	-.45061
				83A -> 90A	.10475
				84A -> 90A	-.35899
				85A -> 90A	.15022

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				86A -> 90A	-.11376
				89A -> 90A	.26808
				80B -> 90B	.45061
				83B -> 90B	-.10475
				84B -> 90B	.35899
				85B -> 90B	-.15022
				86B -> 90B	.11376
				89B -> 90B	-.26808
11	Singlet	4.1989	295.28	80A -> 90A	.11317
				84A -> 90A	.29768
				85A -> 90A	-.31330
				86A -> 90A	.48304
				87A -> 90A	-.17015
				88A -> 90A	-.10949
				80B -> 90B	.11317
				84B -> 90B	.29768
				85B -> 90B	-.31330
				86B -> 90B	.48304
				87B -> 90B	-.17015
				88B -> 90B	-.10949
12	Triplet	4.2236	293.55	80A -> 90A	.17886
				85A -> 90A	.29613
				86A -> 90A	-.55712
				86A -> 91A	.10960
				87A -> 91A	.10587
				88A -> 90A	.13751
				80B -> 90B	-.17886
				85B -> 90B	-.29613
				86B -> 90B	.55712
				86B -> 91B	-.10960
				87B -> 91B	-.10587
				88B -> 90B	-.13751
13	Triplet	4.2357	292.71	83A -> 90A	.14826
				85A -> 90A	-.54946
				85A -> 91A	.11461
				86A -> 90A	-.33417
				83B -> 90B	-.14826
				85B -> 90B	.54946
				85B -> 91B	-.11461
				86B -> 90B	.33417
14	Singlet	4.2369	292.63	83A -> 90A	-.18518
				85A -> 90A	.51448
				86A -> 90A	.37492
				87A -> 90A	.16209
				83B -> 90B	-.18518
				85B -> 90B	.51448
				86B -> 90B	.37492
				87B -> 90B	.16209
15	Singlet	4.2793	289.73	80A -> 90A	.28015
				83A -> 90A	-.21888
				84A -> 90A	.46524
				86A -> 90A	-.25485
				87A -> 90A	.22302

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				80B -> 90B	.28015
				83B -> 90B	-.21888
				84B -> 90B	.46524
				86B -> 90B	-.25485
				87B -> 90B	.22302
16	Triplet	4.2877	289.16	79A -> 90A	-.39278
				83A -> 90A	-.46682
				83A -> 91A	-.14242
				84A -> 90A	-.14718
				85A -> 90A	-.17483
				89A -> 91A	-.10777
				79B -> 90B	.39278
				83B -> 90B	.46682
				83B -> 91B	.14242
				84B -> 90B	.14718
				85B -> 90B	.17483
				89B -> 91B	.10777
17	Singlet	4.3010	288.26	79A -> 90A	-.10176
				83A -> 90A	-.17038
				84A -> 90A	-.29159
				85A -> 90A	-.30994
				86A -> 90A	.11261
				87A -> 90A	.41239
				87A -> 91A	-.14490
				79B -> 90B	.10176
				83B -> 90B	.17038
				84B -> 90B	.29159
				85B -> 90B	.30994
				86B -> 90B	-.11261
				87B -> 90B	-.41239
				87B -> 91B	.14490
18	Singlet	4.3330	286.14	83A -> 90A	.60065
				84A -> 90A	.11169
				87A -> 90A	.25357
				87A -> 91A	-.11484
				83B -> 90B	.60065
				84B -> 90B	.11169
				87B -> 90B	.25357
				87B -> 91B	-.11484
19	Triplet	4.3570	284.56	75A -> 90A	.30983
				76A -> 90A	.16802
				77A -> 90A	-.16507
				79A -> 90A	.10519
				80A -> 90A	.33940
				84A -> 90A	-.34152
				86A -> 91A	-.10380
				87A -> 98A	.16886
				89A -> 91A	-.17205
				75B -> 90B	-.30983
				76B -> 90B	-.16802
				77B -> 90B	.16507
				79B -> 90B	-.10519
				80B -> 90B	-.33940
				84B -> 90B	.34152

				86B -> 91B	.10380
				87B -> 98B	-.16886
				89B -> 91B	.17205
20	Triplet	4.4133	280.93	75A -> 90A	-.29904
				76A -> 90A	-.12355
				77A -> 90A	.16667
				84A -> 94A	.10757
				87A -> 91A	-.11784
				87A -> 98A	-.11547
				89A -> 91A	-.45612
				89A -> 92A	.18948
				75B -> 90B	.29904
				76B -> 90B	.12355
				77B -> 90B	-.16667
				84B -> 94B	-.10757
				87B -> 91B	.11784
				87B -> 98B	.11547
				89B -> 91B	.45612
				89B -> 92B	-.18948

Table 2S. TDDFT Results

2S1: 1 UB3LYP / 6-31G*

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Triplet	2.3583	525.73	63A -> 77A	-.10179
				67A -> 84A	.12181
				74A -> 77A	.17316
				75A -> 77A	.76156
				76A -> 77A	-.30037
				63B -> 77B	.10179
				67B -> 84B	-.12181
				74B -> 77B	-.17316
				75B -> 77B	-.76156
				76B -> 77B	.30037
2	Triplet	3.7786	328.12	71A -> 79A	.36208
				75A -> 77A	.13383
				75A -> 81A	.15390
				76A -> 77A	.34124
				76A -> 79A	.13731
				76A -> 81A	.52509
				71B -> 79B	-.36208
				75B -> 77B	-.13383
				75B -> 81B	-.15390
				76B -> 77B	-.34124
				76B -> 79B	-.13731
				76B -> 81B	-.52509
3	Triplet	3.7947	326.73	64A -> 78A	.11494
				69A -> 78A	.38473
				70A -> 78A	-.10280

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				74A -> 78A	-.40659
				74A -> 79A	-.12424
				74A -> 80A	.48558
				75A -> 80A	-.14073
				64B -> 78B	-.11494
				69B -> 78B	-.38473
				70B -> 78B	.10280
				74B -> 78B	.40659
				74B -> 79B	.12424
				74B -> 80B	-.48558
				75B -> 80B	.14073
4	Singlet	3.8811	319.46	75A -> 77A	.15468
				76A -> 77A	.68601
				75B -> 77B	.15468
				76B -> 77B	.68601
5	Triplet	3.8826	319.33	71A -> 79A	-.23033
				75A -> 77A	.21759
				76A -> 77A	.53170
				76A -> 79A	.12194
				76A -> 81A	-.34658
				71B -> 79B	.23033
				75B -> 77B	-.21759
				76B -> 77B	-.53170
				76B -> 79B	-.12194
				76B -> 81B	.34658
6	Triplet	3.9530	313.64	69A -> 78A	.18495
				70A -> 77A	-.14760
				74A -> 77A	.51856
				74A -> 78A	.31729
				74A -> 80A	.25942
				75A -> 78A	-.11216
				69B -> 78A	.18495
				70B -> 77B	.14760
				74B -> 77B	-.51856
				74B -> 78B	-.31729
				74B -> 80B	-.25942
				75B -> 78B	.11216
7	Triplet	4.0224	308.23	75A -> 79A	.17817
				76A -> 77A	-.16549
				76A -> 79A	.67393
				75B -> 79B	-.17817
				76B -> 77B	.16549
				76B -> 79B	-.67393
8	Singlet	4.0657	304.95	74A -> 77A	.67116
				75A -> 77A	-.18581
				74B -> 77B	.67116
				75B -> 77B	-.18581
9	Triplet	4.0818	303.75	69A -> 78A	.15743
				70A -> 77A	.22161
				74A -> 77A	-.36043
				74A -> 78A	.48493
				74A -> 80A	.22294
				75A -> 78A	-.14626
				69B -> 78B	-.15743

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				70B -> 77B	-.22161
				74B -> 77B	.36043
				74B -> 78B	-.48493
				74B -> 80B	-.22294
				75B -> 78B	.14626
10	Triplet	4.1527	298.56	72A -> 79A	-.13206
				73A -> 77A	.14528
				73A -> 79A	.67551
				73A -> 80A	.10106
				73A -> 81A	-.10975
				72B -> 79B	.13206
				73B -> 77B	-.14528
				73B -> 79B	-.67551
				73B -> 80B	-.10106
				73B -> 81B	.10975
11	Triplet	4.2065	294.74	72A -> 77A	-.14912
				72A -> 78A	-.66053
				73A -> 78A	-.20344
				72B -> 77B	.14912
				72B -> 78B	.66053
				73B -> 78B	.20344
12	Triplet	4.2768	289.90	69A -> 77A	-.10486
				70A -> 77A	-.62670
				74A -> 77A	-.25544
				69B -> 77B	.10486
				70B -> 77B	.62670
				74B -> 77B	.25544
13	Triplet	4.3347	286.02	68A -> 77A	.46248
				71A -> 77A	.12160
				73A -> 77A	.48209
				73A -> 79A	-.12626
				68B -> 77B	-.46248
				71B -> 77B	-.12160
				73B -> 77B	-.48209
				73B -> 79B	.12626
14	Singlet	4.4095	281.17	68A -> 77A	.18928
				70A -> 77A	.16694
				73A -> 77A	.51798
				74A -> 77A	.12208
				75A -> 77A	.31431
				68B -> 77B	.18928
				70B -> 77B	.16694
				73B -> 77B	.51798
				74B -> 77B	.12208
				75B -> 77B	.31431
15	Singlet	4.4189	280.57	70A -> 77A	.17845
				73A -> 77A	-.44336
				74A -> 77A	.14957
				75A -> 77A	.41714
				70B -> 77B	.17845
				73B -> 77B	-.44336
				74B -> 77B	.14957
				75B -> 77B	.41714
16	Triplet	4.4209	280.45	67A -> 77A	-.63775

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				68A -> 82A	-.16173
				69A -> 77A	-.10729
				70A -> 83A	.14327
				75A -> 84A	-.23147
				67B -> 77B	.63775
				68B -> 82B	.16173
				69B -> 77B	.10729
				70B -> 83B	-.14327
				75B -> 84B	.23147
17	Singlet	4.5474	272.65	69A -> 77A	.11300
				70A -> 77A	.58916
				72A -> 77A	.25368
				75A -> 77A	-.20485
				69B -> 77B	.11300
				70B -> 77B	.58916
				72B -> 77B	.25368
				75B -> 77B	-.20485
18	Triplet	4.5607	271.85	68A -> 77A	-.45561
				71A -> 77A	-.12663
				72A -> 77A	.12582
				73A -> 77A	.47802
				75A -> 82A	-.10877
				68A -> 77A	-.45561
				71B -> 77B	.12663
				72B -> 77B	-.12582
				73B -> 77B	-.47802
				75B -> 82B	.10877
19	Singlet	4.7152	262.94	68A -> 77A	-.16660
				70A -> 77A	-.21181
				72A -> 77A	.61432
				72A -> 78A	.12366
				75A -> 77A	.10432
				68B -> 77B	-.16660
				70B -> 77B	-.21181
				72B -> 77B	.61432
				72B -> 78B	.12366
				75B -> 77B	.10432
20	Triplet	4.7391	261.62	68A -> 77A	.10455
				69A -> 78A	-.10834
				72A -> 77A	.64962
				72A -> 78A	-.11584
				68B -> 77B	-.10455
				69B -> 78B	.10834
				72B -> 77B	-.64962
				72B -> 78B	.11584

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2S2: 2 UB3LYP / 6-31G* Rotational Isomer #1

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Triplet	2.3354	530.88	87A -> 95A	-.33661
				94A -> 95A	-.62601
				94A -> 96A	.12135
				87B -> 95B	.33661
				94B -> 95B	.62601
				94B -> 96B	-.12135
2	Triplet	2.3428	529.22	73A -> 95A	-.10097
				85A -> 95A	.11345
				86A -> 95A	-.12559
				87A -> 95A	.73397
				94A -> 95A	-.28853
				73B -> 95B	.10097
				85B -> 95B	-.11345
				86B -> 95B	.12559
				87B -> 95B	-.73397
				94B -> 95B	.28853
3	Singlet	2.3482	528.00	94A -> 95A	.69918
				94B -> 95B	.69918
4	Triplet	2.5462	486.93	93A -> 95A	.64946
				93A -> 96A	-.23317
				93B -> 95B	-.64946
				93B -> 96B	.23317
5	Singlet	2.5740	481.67	93A -> 95A	.69363
				93A -> 96A	-.12165
				93B -> 95B	.69363
				93B -> 96B	-.12165
6	Triplet	2.7152	456.62	93A -> 95A	.16019
				93A -> 96A	.10300
				93A -> 97A	-.16259
				94A -> 95A	.14352
				94A -> 96A	.53689
				94A -> 97A	-.33153
				93B -> 95B	-.16019
				93B -> 96B	-.10300
				93B -> 97B	.16259
				94B -> 95B	-.14352
				94B -> 96B	-.53689
				94B -> 97B	.33153
7	Triplet	2.7332	453.63	92A -> 95A	.63875
				92A -> 96A	-.23949
				94A -> 96A	.10290
				92B -> 95B	-.63875
				92B -> 96B	.23949
				94B -> 96B	-.10290
8	Singlet	2.7691	447.74	92A -> 95A	.67819
				94A -> 96A	.11528
				92B -> 95B	.67819
				94B -> 96B	.11528

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9	Triplet	2.8011	442.63	93A -> 95A	-.15113
				93A -> 96A	-.31707
				94A -> 96A	.39574
				94A -> 97A	.44687
				93B -> 95B	.15113
				93B -> 96B	.31707
				94B -> 96B	-.39574
				94B -> 97B	-.44687
10	Singlet	2.8041	442.16	92A -> 95A	-.12282
				94A -> 96A	.68347
				92B -> 95B	-.12282
				94B -> 96B	.68347
11	Triplet	2.8419	436.27	93A -> 95A	.13376
				93A -> 96A	.53097
				93A -> 97A	.25178
				94A -> 96A	.13001
				94A -> 97A	.31210
				93B -> 95B	-.13376
				93B -> 96B	-.53097
				93B -> 97B	-.25178
				94B -> 96B	-.13001
				94B -> 97B	-.31210
12	Singlet	2.8744	431.33	94A -> 97A	.68683
				94B -> 97B	.68683
13	Triplet	2.9361	422.28	91A -> 95A	-.31131
				91A -> 97A	-.12430
				93A -> 97A	0.54011
				94A -> 97A	-.26774
				91B -> 95B	.31131
				91B -> 97B	.12430
				93B -> 97B	-0.54011
				94B -> 97B	.26774
14	Singlet	2.9491	420.41	91A -> 95A	.32867
				91A -> 96A	-.11154
				93A -> 95A	.11141
				93A -> 96A	.58165
				91B -> 95B	.32867
				91B -> 96B	-.11154
				93B -> 95B	.11141
				93B -> 96B	.58165
15	Triplet	2.9665	417.94	90A -> 95A	.39667
				90A -> 96A	-.19915
				91A -> 95A	-.34418
				92A -> 95A	-.19482
				92A -> 96A	-.31395
				93A -> 96A	.10603
				93A -> 97A	-.14470
				90B -> 95B	-.39667
				90B -> 96B	.19915
				91B -> 95B	.34418
				92B -> 95B	.19482
				92B -> 96B	.31395

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				93B -> 96B	-.10603
				93B -> 97B	.14470
16	Singlet	2.9812	415.89	91A -> 95A	.61495
				93A -> 96A	-.32256
				91B -> 95B	.61495
				93B -> 96B	-.32256
17	Triplet	2.9850	415.35	90A -> 95A	.29282
				90A -> 96A	-.13214
				91A -> 95A	.50613
				92A -> 95A	-.10150
				92A -> 96A	-.20125
				93A -> 96A	-.12327
				93A -> 97A	.24752
				90B -> 95A	.29282
				90B -> 96A	-.13214
				91B -> 95B	-.50613
				92B -> 95B	.10150
				92B -> 96B	.20125
				93B -> 96B	.12327
				93B -> 97B	-.24752
18	Singlet	3.0175	410.88	90A -> 95A	.62718
				93A -> 97A	-.28669
				90B -> 95B	.62718
				93B -> 97B	-.28669
19	Triplet	3.0570	405.57	90A -> 95A	.48469
				92A -> 95A	.15099
				92A -> 96A	.46480
				90B -> 95B	-.48469
				92B -> 95B	-.15099
				92B -> 96B	-.46480
20	Singlet	3.0692	403.96	90A -> 95A	.29837
				92A -> 96A	.25952
				92A -> 97A	-.10199
				93A -> 97A	.54557
				90B -> 95B	.29837
				92B -> 96B	.25952
				92B -> 97B	-.10199
				93B -> 97B	.54557

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2S3: 3 UB3LYP / 6-31G* Rotational Isomer #1

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Doublet	0.7211	1719.40	73B -> 93B	-.28659
				75B -> 93B	-.11160
				76B -> 93B	-.17682
				78B -> 93B	-.14431
				85B -> 93B	-.25830
				87B -> 93B	-.11054
				90B -> 93B	.69306
				91B -> 93B	.12590
				92B -> 93B	.59306
2	Doublet	0.9455	1311.35	73B -> 93B	-.12025
				75B -> 93B	.29042
				77B -> 93B	-.20485
				78B -> 93B	.11415
				84B -> 93B	.20509
				89B -> 93B	-.49006
				90B -> 93B	.13727
				91B -> 93B	.69160
				92B -> 93B	-.26149
3	Doublet	0.9615	1289.48	73B -> 93B	-.25567
				74B -> 93B	.22748
				77B -> 93B	.17231
				78B -> 93B	.15521
				89B -> 93B	.10414
				90B -> 93B	.65131
				91B -> 93B	-.23188
				92B -> 93B	-.60621
4	Doublet	1.4669	845.18	75B -> 93B	-.10597
				84B -> 93B	-.32820
				89B -> 93B	.68758
				91B -> 93B	.60001
5	Doublet	1.5601	794.71	73B -> 93B	-.19432
				76B -> 93B	.52347
				77B -> 93B	-.27207
				78B -> 93B	-.26779
				79B -> 93B	.21027
				80B -> 93B	.15657
				81B -> 93B	-.23651
				85B -> 93B	.50054
				86B -> 93B	-.17142
				87B -> 93B	.31371
				90B -> 93B	.14233
				92B -> 93B	.10535
6	Doublet	2.0786	596.46	74B -> 93B	-.10900
				75B -> 93B	.37451
				76B -> 93B	-.12844
				77B -> 93B	-.29877
				78B -> 93B	.21376
				79B -> 93B	-.11314

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				80B -> 93B	-.11154
				84B -> 93B	.59716
				85B -> 93B	.12992
				89B -> 93B	.49180
				91B -> 93B	-.15034
7	Doublet	2.2370	554.25	72B -> 93B	-.10049
				73B -> 93B	-.13842
				74B -> 93B	.35776
				75B -> 93B	.20851
				76B -> 93B	.18310
				77B -> 93B	.29120
				78B -> 93B	.58180
				79B -> 93B	-.21726
				81B -> 93B	.17865
				86B -> 93B	.10247
				87B -> 93B	.26734
				92B -> 93B	.37900
8	Quartet	2.3490	527.82	89A -> 94A	-.82180
				89A -> 95A	-.10946
				88B -> 94B	.82530
				88B -> 95B	.10120
9	Doublet	2.5593	484.45	73B -> 93B	-.11319
				78B -> 93B	-.13501
				85B -> 93B	-.30883
				86B -> 93B	.26678
				87B -> 93B	.64312
				88B -> 93B	-.58553
10	Doublet	2.5750	481.49	73B -> 93B	-.26625
				84B -> 93B	.10184
				85B -> 93B	-.41448
				86B -> 93B	-.14338
				87B -> 93B	.40561
				88B -> 93B	.72308
				90B -> 93B	-.13271
11	Doublet	2.6073	475.52	68B -> 93B	-.13305
				73B -> 93B	-.71633
				74B -> 93B	.27203
				76B -> 93B	.11807
				79B -> 93B	.10484
				80B -> 93B	.18047
				81B -> 93B	-.15725
				85B -> 93B	-.12057
				86B -> 93B	.17839
				87B -> 93B	-.43628
				88B -> 93B	-.14842
				90B -> 93B	-.27874
12	Doublet	2.6507	467.74	85B -> 93B	.23117
				86B -> 93B	.90143
				88B -> 93B	.32646
13	Doublet	3.2576	380.59	74B -> 93B	.17080
				75B -> 93B	-.44302
				76B -> 93B	.15722
				77B -> 93B	.38688

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				78B -> 93B	-.14476
				80B -> 93B	.17006
				81B -> 93B	.14661
				84B -> 93B	.60609
				91B -> 93B	.13338
14	Doublet	3.3141	374.11	73B -> 93B	.40485
				75B -> 93B	.14988
				76B -> 93B	.62142
				77B -> 93B	-.12309
				78B -> 93B	.12463
				80B -> 93B	.11621
				81B -> 93B	-.15448
				85B -> 93B	-.46335
				87B -> 93B	-.14520
				90B -> 93B	.13925
15	Quartet	3.6164	342.83	81A -> 96A	-.16816
				86A -> 96A	.12076
				87A -> 95A	.24275
				87A -> 96A	.59120
				87A -> 98A	-.21102
				90A -> 96A	-.19270
				81B -> 96B	.16702
				86B -> 96B	-.18698
				87B -> 95B	-.25171
				87B -> 96B	-.55655
				87B -> 98B	.20290
				89B -> 96B	.14396
16	Doublet	3.6496	339.72	80A -> 95A	-.10191
				86A -> 94A	-.21882
				86A -> 95A	.57068
				86A -> 97A	-.20570
				87A -> 95A	-.12902
				80B -> 95B	.10130
				85B -> 95B	-.14301
				86B -> 94B	.20463
				86B -> 95B	-.52427
				86B -> 96B	.21668
				86B -> 97B	.19717
				87B -> 95B	.17941
				92B -> 94B	.30621
17	Doublet	3.6793	336.98	86A -> 95A	-.17340
				86A -> 97A	.14366
				86B -> 95B	.16504
				86B -> 97B	-.13667
				91B -> 94B	-.12133
				92B -> 94B	.91022
				92B -> 95B	-.10792
18	Doublet	3.6886	336.13	83B -> 93B	.99193
19	Doublet	3.7165	333.60	90B -> 94B	.20114
				91B -> 94B	.91926
				91B -> 95B	-.17769
				91B -> 96B	.11921
				92B -> 94B	.17015

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20	Doublet	3.7979	326.45	79A -> 95A	.11538
				80A -> 95A	.23126
				86A -> 94A	-.13069
				86A -> 95A	.13597
				86A -> 97A	.42455
				91A -> 94A	.11199
				92A -> 94A	-.18094
				93A -> 94A	.53727
				93A -> 95A	-.11997
				80B -> 95B	-.23595
				80B -> 96B	.11089
				85B -> 95B	-.10701
				85B -> 97B	-.14395
				86B -> 94B	.10577
				86B -> 95B	-.11596
				86B -> 97B	-.39491
				87B -> 97B	.11666
				91B -> 94B	.16916
				92B -> 94B	-.10307

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2S4: 4 UB3LYP / 6-31G* Rotational Isomer #1

State	Multiplicity	E (eV)	E (nm)	Configuration	Expansion Coeff.
1	Triplet	2.3468	528.30	85A -> 90A	.12715
				87A -> 90A	-.80410
				87A -> 91A	-.15793
				85B -> 90B	-.12715
				87B -> 90B	.80410
				87B -> 91B	.15793
2	Triplet	3.6336	341.22	78A -> 92A	-.10894
				83A -> 92A	-.16239
				84A -> 90A	.14824
				84A -> 91A	-.45840
				84A -> 92A	.44241
				84A -> 94A	.19197
				78B -> 92B	.10894
				83B -> 92B	.16239
				84B -> 90B	-.14824
				84B -> 91B	.45840
				84B -> 92B	-.44241
				84B -> 94B	-.19197
3	Triplet	3.6493	339.74	83A -> 90A	-.24052
				83A -> 91A	.48117
				83A -> 92A	.42720
				83A -> 93A	-.18650
				84A -> 92A	.15716
				83B -> 90B	.24052
				83B -> 91B	-.48117
				83B -> 92B	-.42720
				83B -> 93B	.18650
				84B -> 92B	-.15716
4	Triplet	3.8229	324.32	77A -> 90A	.10411
				77A -> 91A	-.25995
				77A -> 92A	-.24067
				77A -> 93A	-.11289
				83A -> 90A	.14465
				83A -> 91A	-.13527
				83A -> 93A	-.57637
				83A -> 94A	.13837
				84A -> 93A	-.14830
				77B -> 90B	-.10411
				77B -> 91B	.25995
				77B -> 92B	.24067
				77B -> 93B	.11289
				83B -> 90B	-.14465
				83B -> 91B	.13527
				83B -> 93B	.57637
				83B -> 94B	-.13837
				84B -> 93B	.14830
5	Triplet	3.8742	320.02	78A -> 91A	-.24931
				78A -> 92A	.28748

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				78A -> 94A	-.14080
				83A -> 94A	.11234
				84A -> 90A	.16826
				84A -> 92A	.15229
				84A -> 93A	-.11269
				84A -> 94A	-.50242
				86A -> 94A	-.10883
				89A -> 90A	.11035
				78B -> 91B	.24931
				78B -> 92B	-.28748
				78B -> 94B	.14080
				83B -> 94B	-.11234
				84B -> 90B	-.16826
				84B -> 92B	-.15229
				84B -> 93B	.11269
				84B -> 94B	.50242
				86B -> 94B	.10883
				89B -> 90B	-.11035
6	Singlet	4.0589	305.46	86A -> 90A	.11198
				89A -> 90A	.67790
				89A -> 91A	-.10979
				86B -> 90B	.11198
				89B -> 90B	.67790
				89B -> 91B	-.10979
7	Triplet	4.0630	305.15	80A -> 90A	-.19527
				84A -> 90A	-.13908
				84A -> 91A	-.10631
				84A -> 94A	-.11845
				86A -> 90A	-.10960
				89A -> 90A	-.60577
				80B -> 90B	.19527
				84B -> 90B	.13908
				84B -> 91B	.10631
				84B -> 94B	.11845
				86B -> 90B	.10960
				89B -> 90B	.60577
8	Triplet	4.0894	303.19	86A -> 90A	-.10474
				88A -> 90A	-.66909
				88A -> 91A	.12382
				86B -> 90B	.10474
				88B -> 90B	.66909
				88B -> 91B	-.12382
9	Singlet	4.0910	303.06	85A -> 90A	-.10359
				86A -> 90A	.10728
				88A -> 90A	.67739
				88A -> 91A	-.12043
				85B -> 90B	-.10359
				86B -> 90B	.10728
				88B -> 90B	.67739
				88B -> 91B	-.12043
10	Triplet	4.1057	301.98	80A -> 90A	-.45061
				83A -> 90A	.10475
				84A -> 90A	-.35899
				85A -> 90A	.15022

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				86A -> 90A	-.11376
				89A -> 90A	.26808
				80B -> 90B	.45061
				83B -> 90B	-.10475
				84B -> 90B	.35899
				85B -> 90B	-.15022
				86B -> 90B	.11376
				89B -> 90B	-.26808
11	Singlet	4.1989	295.28	80A -> 90A	.11317
				84A -> 90A	.29768
				85A -> 90A	-.31330
				86A -> 90A	.48304
				87A -> 90A	-.17015
				88A -> 90A	-.10949
				80B -> 90B	.11317
				84B -> 90B	.29768
				85B -> 90B	-.31330
				86B -> 90B	.48304
				87B -> 90B	-.17015
				88B -> 90B	-.10949
12	Triplet	4.2236	293.55	80A -> 90A	.17886
				85A -> 90A	.29613
				86A -> 90A	-.55712
				86A -> 91A	.10960
				87A -> 91A	.10587
				88A -> 90A	.13751
				80B -> 90B	-.17886
				85B -> 90B	-.29613
				86B -> 90B	.55712
				86B -> 91B	-.10960
				87B -> 91B	-.10587
				88B -> 90B	-.13751
13	Triplet	4.2357	292.71	83A -> 90A	.14826
				85A -> 90A	-.54946
				85A -> 91A	.11461
				86A -> 90A	-.33417
				83B -> 90B	-.14826
				85B -> 90B	.54946
				85B -> 91B	-.11461
				86B -> 90B	.33417
14	Singlet	4.2369	292.63	83A -> 90A	-.18518
				85A -> 90A	.51448
				86A -> 90A	.37492
				87A -> 90A	.16209
				83B -> 90B	-.18518
				85B -> 90B	.51448
				86B -> 90B	.37492
				87B -> 90B	.16209
15	Singlet	4.2793	289.73	80A -> 90A	.28015
				83A -> 90A	-.21888
				84A -> 90A	.46524
				86A -> 90A	-.25485
				87A -> 90A	.22302

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				80B -> 90B	.28015
				83B -> 90B	-.21888
				84B -> 90B	.46524
				86B -> 90B	-.25485
				87B -> 90B	.22302
16	Triplet	4.2877	289.16	79A -> 90A	-.39278
				83A -> 90A	-.46682
				83A -> 91A	-.14242
				84A -> 90A	-.14718
				85A -> 90A	-.17483
				89A -> 91A	-.10777
				79B -> 90B	.39278
				83B -> 90B	.46682
				83B -> 91B	.14242
				84B -> 90B	.14718
				85B -> 90B	.17483
				89B -> 91B	.10777
17	Singlet	4.3010	288.26	79A -> 90A	-.10176
				83A -> 90A	-.17038
				84A -> 90A	-.29159
				85A -> 90A	-.30994
				86A -> 90A	.11261
				87A -> 90A	.41239
				87A -> 91A	-.14490
				79B -> 90B	.10176
				83B -> 90B	.17038
				84B -> 90B	.29159
				85B -> 90B	.30994
				86B -> 90B	-.11261
				87B -> 90B	-.41239
				87B -> 91B	.14490
18	Singlet	4.3330	286.14	83A -> 90A	.60065
				84A -> 90A	.11169
				87A -> 90A	.25357
				87A -> 91A	-.11484
				83B -> 90B	.60065
				84B -> 90B	.11169
				87B -> 90B	.25357
				87B -> 91B	-.11484
19	Triplet	4.3570	284.56	75A -> 90A	.30983
				76A -> 90A	.16802
				77A -> 90A	-.16507
				79A -> 90A	.10519
				80A -> 90A	.33940
				84A -> 90A	-.34152
				86A -> 91A	-.10380
				87A -> 98A	.16886
				89A -> 91A	-.17205
				75B -> 90B	-.30983
				76B -> 90B	-.16802
				77B -> 90B	.16507
				79B -> 90B	-.10519
				80B -> 90B	-.33940
				84B -> 90B	.34152

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				86B -> 91B	.10380
				87B -> 98B	-.16886
				89B -> 91B	.17205
20	Triplet	4.4133	280.93	75A -> 90A	-.29904
				76A -> 90A	-.12355
				77A -> 90A	.16667
				84A -> 94A	.10757
				87A -> 91A	-.11784
				87A -> 98A	-.11547
				89A -> 91A	-.45612
				89A -> 92A	.18948
				75B -> 90B	.29904
				76B -> 90B	.12355
				77B -> 90B	-.16667
				84B -> 94B	-.10757
				87B -> 91B	.11784
				87B -> 98B	.11547
				89B -> 91B	.45612
				89B -> 92B	-.18948