

Article

# Supplementary Materials for Electronically Excited States of Closed-Shell, Cyano-Functionalized Polycyclic Aromatic Hydrocarbon Anions

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**1 Supplementary Materials:**

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**Table 1.** The oscillator strengths for each of the EOM-CCSD/apVDZ+6s6p2d dipole bound and EOM-CCSD/apVDZ valence excited states.

Benzonitrile	Oscillator Strengths	
	$2\ ^1A'/2\ ^1A_1$	$1\ ^1A''/1\ ^1B_1$
2	$2 \times 10^{-3}$	$8 \times 10^{-6}$
3	$2 \times 10^{-3}$	$2 \times 10^{-4}$
4	$3 \times 10^{-3}$	$6 \times 10^{-5}$
1-Cyanonaph.		
2	$2 \times 10^{-3}$	$2 \times 10^{-6}$
3	$2 \times 10^{-3}$	$7 \times 10^{-7}$
4	$4 \times 10^{-7}$	$3 \times 10^{-8}$
5	$3 \times 10^{-3}$	$7 \times 10^{-8}$
6	$3 \times 10^{-3}$	$> 1 \times 10^{-6}$
7	$2 \times 10^{-3}$	$4 \times 10^{-6}$
8	$4 \times 10^{-4}$	$5 \times 10^{-6}$
2-Cyanonaph.		
1	$1 \times 10^{-4}$	$4 \times 10^{-6}$
3	$8 \times 10^{-4}$	$2 \times 10^{-4}$
4	$4 \times 10^{-4}$	$5 \times 10^{-6}$
5	$3 \times 10^{-3}$	$5 \times 10^{-7}$
6	$6 \times 10^{-3}$	$3 \times 10^{-3}$
7	$5 \times 10^{-3}$	$5 \times 10^{-4}$
8	$1 \times 10^{-3}$	$3 \times 10^{-6}$
1-Cyanoanthra.		
2	$3 \times 10^{-4}$	$> 1 \times 10^{-6}$
3	$2 \times 10^{-4}$	$1 \times 10^{-3}$
4	$3 \times 10^{-3}$	$6 \times 10^{-4}$
5	$4 \times 10^{-3}$	$7 \times 10^{-4}$
6	$4 \times 10^{-3}$	$2 \times 10^{-3}$
2-Cyanoantha.		
1	$2 \times 10^{-4}$	$1 \times 10^{-3}$
3	$2 \times 10^{-3}$	$2 \times 10^{-3}$
4	$4 \times 10^{-3}$	$7 \times 10^{-4}$
5	$5 \times 10^{-3}$	$2 \times 10^{-3}$
6	$3 \times 10^{-3}$	$1 \times 10^{-3}$
7	$2 \times 10^{-3}$	$5 \times 10^{-4}$
8	$3 \times 10^{-3}$	$9 \times 10^{-4}$
9	$1 \times 10^{-3}$	$1 \times 10^{-3}$
10	$3 \times 10^{-4}$	$4 \times 10^{-4}$
3-Cyanoantha.		
1	$3 \times 10^{-3}$	$1 \times 10^{-3}$
2	$5 \times 10^{-5}$	$1 \times 10^{-3}$
4	$4 \times 10^{-4}$	$5 \times 10^{-4}$
5	$5 \times 10^{-4}$	$8 \times 10^{-4}$
6	$4 \times 10^{-4}$	$1 \times 10^{-3}$
7	$2 \times 10^{-3}$	$5 \times 10^{-4}$
8	$5 \times 10^{-3}$	$1 \times 10^{-3}$
9	$6 \times 10^{-3}$	$8 \times 10^{-4}$
10	$1 \times 10^{-3}$	$7 \times 10^{-4}$

**Table 2.** Anion derivative emission energies and eBE, neutral radical dipole moments, and neutral radical and anion relative energies for the cyanonaphthalene deprotonated derivatives

1-Cyanonaph.	Excited States		eBE (eV)
	2 <sup>1</sup> A'	1 <sup>1</sup> A''	
2	1.6249	1.6530	1.6445
3	1.4885	1.5069	1.4975
4	1.5852	1.6010	1.5910
5	1.4198	1.4352	1.4230
6	1.2714	1.2909	1.2799
7	1.2433	1.2723	1.2637
8	1.2759	1.2982	1.2894
2-Cyanonaph.			
1	1.7219	1.7421	1.7339
3	1.5706	1.3795	1.5795
4	1.5261	1.5423	1.5332
5	1.4297	1.4262	1.4500
6	1.3901	1.4188	1.4024
7	1.3362	1.2206	1.3622
8	1.4506	1.4887	1.4800

**Table 3.** Anion emission derivatives vertical excitation energies and eBE, neutral radicals dipole moments, and neutral radicals and anions relative energies for cyanoanthracene deprotonated derivatives

1-Cyanonaph.	Excited States		eBE (eV)
	2 <sup>1</sup> A'	1 <sup>1</sup> A''	
2	1.3991	—	1.4022
3	1.4173	—	1.4207
4	—	—	1.4173
5	—	—	1.5692
6 <sup>a</sup>	1.8616	—	1.8750
2-Cyanoanthra.			
1	1.5780	1.0664	1.5844
3	1.7711	1.1758	1.7952
4	1.6239	0.8628	1.6338
5	1.7177	1.1466	1.7253
6	1.7191	1.1747	1.7239
7	1.4189	0.8851	1.4261
8	1.3191	0.8030	1.3304
9	1.2994	0.8159	1.3248
10	1.3274	0.8080	1.3447
3-Cyanoanthra.			
1	1.7883	1.8134	1.8047
2	1.8820	1.3154	1.8860
4	1.6914	1.0020	1.6936
5	1.6473	1.0989	1.6497
6	1.7136	1.1867	1.7266
7	1.4656	0.9149	1.4997
8	1.4294	0.9200	1.4525
9	1.3802	0.8231	1.4222
10	1.4756	0.9353	1.5163

<sup>a</sup>1-cyanoanthracene isomer 6 is C<sub>2v</sub>.