Supplemental Information

Table S1: Redox potentials of 9-methyl-2AP calculated with different basis sets using the B3LYP functional. ACN (ε = 35.94) was used as the solvent.

Species/Theory	E_{PCM} kcal/mol	$E_{THERMAL}$ kcal/mol	S cal/(mol •K)	E^{o}_{OX} V	E^{o}_{RED} V
6-31G(d, p)					
Neutral	-317935	92.672	93.662		
Cation radical	-317807	92.321	93.814	1.160	
Anion radical	-317965	90.548	98.646		-2.910
6-31+G(d, p)					
Neutral	-317950	92.369	93.014		
Cation radical	-317816	92.093	93.425	1.429	
Anion radical	-317991	90.296	96.142		-2.422
6-31++G(d, p)					
Neutral	-317950	93.37	93.019		
Cation radical	-317816	92.096	93.414	1.429	
Anion radical	-317992	90.29	96.191		-2.421
6-311+G(2d, 2p)					
Neutral	-318025	92.19	92.943		
Cation radical	-317891	91.923	93.489	1.425	
Anion radical	-318067	90.166	95.719		-2.400

Table S2: One electron oxidation and reductions potentials of 9-methyl-2AP calculated at the B3LYP/6-31+G (d,p) level for the solvents ACN and DMF

		Species	E_{PCM} kcal/mol	$E_{THERMAL}$ kcal/mol	S cal/(mol K)	E°_{OX} V	E°_{RED} V
2AP	ACN	Neutral	-317949.7625	92.369	93.014		
		Cation radical	-317815.8629	92.093	93.425	1.429	
		Anion radical	-317991.4483	90.296	98.142		-2.422
	DMF	Neutral	-317949.7895	92.370	93.047		
		Cation radical	-317815.9395	92.092	93.458	1.427	
		Anion radical	-317991.5207	90.297	96.147		-2.420

Complete Reference 45

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, J.; T. Vreven, K. N. K.; J. C. Burant, J. M. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.;

Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision A.1*, Gaussian, Inc.: Pittsburgh, PA, 2003.