Supporting Information for

A Crystalline Phosphaalkene Radical Anion

Xiaobo Pan,[†] Xingyong Wang,[†] Yue Zhao,[†] Yunxia Sui,[‡] and Xinping Wang[†]*

[†]State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China. [‡]Centre of Modern Analysis, Nanjing University, Nanjing 210093, China.

E-mail: xpwang@nju.edu.cn

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Experimental Section

All experiments were carried out under a nitrogen atmosphere by using standard Schlenk techniques and a glovebox. Solvents were dried prior to use. The phosphaalkene **1** was synthesized according to literature methods.[s1] Cyclic voltammetry was performed on an IM6ex electrochemical workstation with platinum as the working and a saturated calomel electrode as reference. Freshly distilled THF was used as a solvent and $^{n}Bu_4NPF_6$ (10^{-1}M) was used as electrolyte. EPR spectra were obtained using Bruker EMX-10/12 variable-temperature apparatus. UV-Vis spectra were recorded on Lambda 750 spectrometer. Element analyses were performed at Shanghai Institute of Organic Chemistry, the Chinese Academy of Sciences. X-ray crystal structures were obtained by using Bruker APEX DUO CCD detectors. CCDC-1007154 ($[Li(DME)_3]^+\cdot\mathbf{1}^{\bullet-}$) and 1006489 ($[K(THF)_3]^+\cdot\mathbf{1}^{\bullet-}$) contain the supplementary crystallographic data for this paper.

Table S1. Crystal Data and Structure Refinement

	$[K(THF)_3]^+\cdot\mathbf{1}^{\bullet-}$	$[Li(DME)_3]^+\cdot\mathbf{1}^{\bullet-}$	$[K(THF)_4]^+\cdot[\mathbf{1H}]^-$
formula	$C_{55}H_{85}KO_4P$	$C_{51}H_{83}LiO_6P$	$C_{55}H_{86}KO_4P$
Mr [g mol^{-1}]	880.30	830.08	881.31
crystal system	*Orthorhombic*	*Triclinic*	*Monoclinic*
space group	*Pna2(1)*	*P-1*	*P2(1)/n*
Z	4	2	4
μ (mm^{-1})	0.174	0.098	0.173
a (Å)	33.185(3)	11.2419(12)	9.996(3)
b (Å)	10.8157(9)	11.4340(12)	20.129(6)
c (Å)	14.5739(12)	20.378(2)	26.154(8)
α (^{o})		88.2750(10)	
β (^{o})		89.862(2)	93.930(5)
γ (^{o})		76.552(2)	
V [Å^3]	5230.8(7)	2546.4(5)	5250(3)
R1 (I>2σ(*I*))	0.0441	0.0473	
wR2 (all data)	0.1039	0.1110	

S1. Decken, A.; Claire, J. C.; Clyburne, J. A. C.; Cowley, A. H. *Inorg. Chem*. **1997**, *36*, 3741.

Synthesis of $[Li(DME)_3]^+ \cdot \mathbf{1}^{\bullet-}$:

Under anaerobic and anhydrous conditions, a mixture of phosphaalkene **1** (0.138 g, 0.250 mmol) and excess lithium (0.013 g, 1.85 mmol) in DME (≈ 30 mL) was stirred at room temperature for 1 day. The resultant purple solution was filtered and the filtrate was then concentrated and stored at -30 ^{o}C for 1 day in glovebox to afford purple X-ray-quality crystals of phosphaalkene radical anion salts. Yield: 0.116 g, 56.0 %; m.p.: 65 ^{o}C, turn yellow; UV-Vis (DME): λ_{max} = 578, 504 and 366 nm; elemental analysis calcd (%): C, 73.78； H, 10.10; found: C 73.64, H 10.61.

Synthesis of $[K(THF)_3]^+ \cdot \mathbf{1}^{\bullet-}$:

Under anaerobic and anhydrous conditions, a mixture of phosphaalkene **1** (0.165 g, 0.298 mmol) and excess potassium (0.034 g, 0.870 mmol) in THF (≈ 50 mL) was stirred at room temperature for 1 day. The resultant purple solution was filtered and the filtrate was then concentrated and stored at around -20 ^{o}C for 1 day to afford purple X-ray-quality crystals of phosphaalkene radical anion salts. Yield: 0.097 g, 36.7 %; m.p.: 78 ^{o}C, turn yellow; UV-vis (THF): λ_{max} = 572, 502 and 366 nm. $[K(THF)_3]^+ \cdot \mathbf{1}^{\bullet-}$ gradually decomposes in the solid state in the glove box with the color changes from purple to pale yellow, which together with solvates prevents accurate elemental analysis.

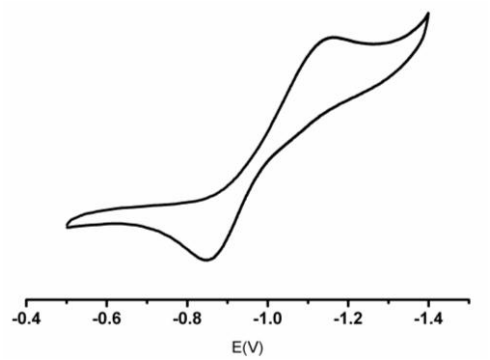


Figure S1. Cyclic voltammogram of **1** (1×10^{-3} M) in THF, containing 0.1 M $^{n}Bu_4NPF_6$, measured at 100 mV s^{-1} at 25 ^{o}C.

Table S2. Experimental and Calculated Structural Parameters for Phosphaalkene **1** and related Species.

Experimental			
	1[S1]	$[K(THF)_3]^+\cdot\mathbf{1}^{\bullet-}$	$[Li(DME)_3]^+\cdot\mathbf{1}^{\bullet-}$
P1–C1 (Å)	1.681	1.757(3)	1.754(2)
P1–C22 (Å)	1.850	1.854(3)	1.871(2)
C1-C2 (Å)	1.482	1.452(5)	1.448(3)
C1-C5 (Å)	1.484	1.420(4)	1.452(3)
C2-C3 (Å)	1.404	1.432(5)	1.430(3)
C3-C4 (Å)	1.458	1.427(5)	1.445(3)
C4-C5 (Å)	1.400	1.435(5)	1.430(3)
C22-C27 (Å)	1.426	1.417(5)	1.431(3)
C22-C23 (Å)	1.421	1.450(4)	1.440(3)
C23-C24 (Å)	1.388	1.374(4)	1.397(3)
C24-C25 (Å)	1.376	1.388(5)	1.385(3)
C25-C26 (Å)	1.382	1.370(5)	1.386(3)
C26-C27 (Å)	1.387	1.401(4)	1.403(3)
∠C1–P1–C22 (°)	107.0	105.91(14)	106.90(10)
∠C2–C1–P1 (°)	136.1	134.5(2)	134.58(16)
∠C5–C1–P1 (°)	119.2	119.9(2)	120.16(16)
Calculated			
	1	$[K(THF)_3]^+\cdot\mathbf{1}^{\bullet-}$	$\mathbf{1}^{\bullet-}$
P1–C1 (Å)	1.693	1.771	1.765
P1–C22 (Å)	1.854	1.871	1.875
C1-C2 (Å)	1.472	1.445	1.444
C1-C5 (Å)	1.482	1.450	1.448
C2-C3 (Å)	1.416	1.438	1.435
C3-C4 (Å)	1.460	1.442	1.442
C4-C5 (Å)	1.407	1.429	1.425
C22-C27 (Å)	1.425	1.428	1.429
C22-C23 (Å)	1.430	1.432	1.433
C23-C24 (Å)	1.396	1.396	1.398
C24-C25 (Å)	1.392	1.392	1.391
C25-C26 (Å)	1.388	1.388	1.387
C26-C27 (Å)	1.401	1.403	1.403
∠C1–P1–C22 (°)	107.7	106.5	106.4
∠C2–C1–P1 (°)	135.2	135.0	135.2
∠C5–C1–P1 (°)	119.5	119.5	119.2

S1. Decken, A.; Claire, J. C.; Clyburne, J. A. C.; Cowley, A. H. *Inorg. Chem*. **1997**, *36*, 3741.

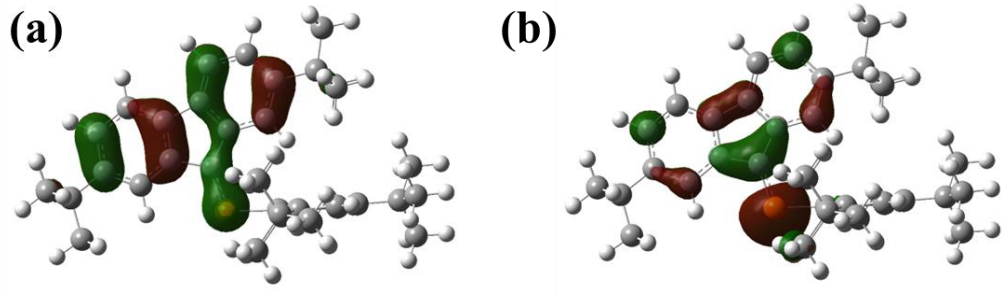


Figure S2. HOMO (a) and LUMO (b) of **1** calculated at the PBE0/6-31G(d) level.

Table S3. Selected Mulliken atomic spin densities for some atoms in $\mathbf{1}^{\bullet-}$

P1	0.594
C2	0.108
C3	-0.003
C4	0.074
C5	0.050
C6	0.022
C7	0.042
C9	-0.016
C10	0.070
C12	-0.035
C14	-0.050
C16	0.094
C18	-0.027
C19	0.067
C47	-0.016
C56	0.013
C86	0.012

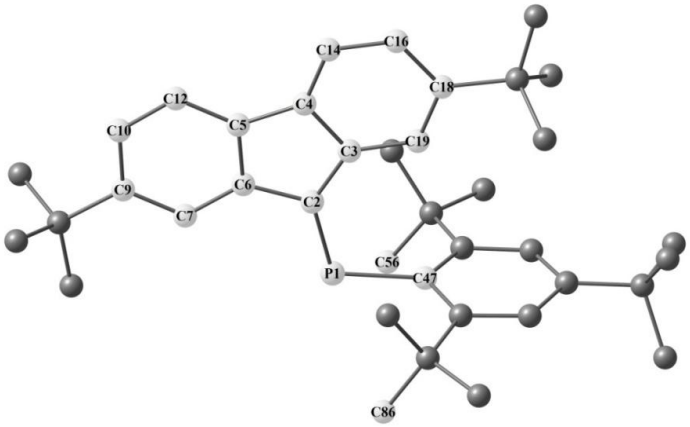
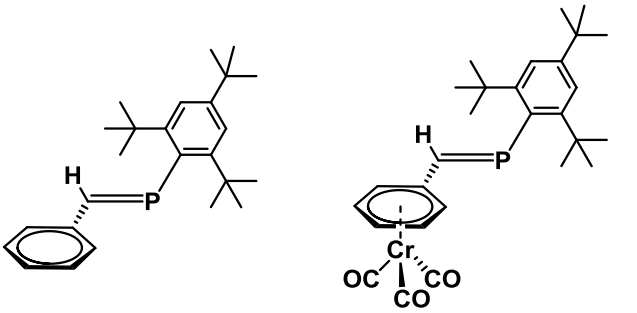
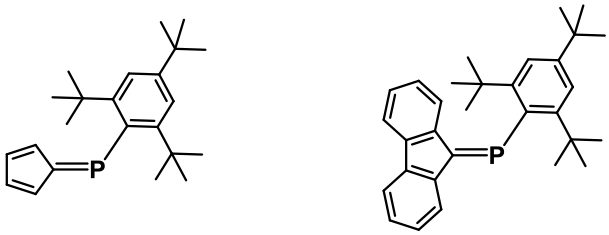


Table S4. Experimental EPR parameters and spin densities obtained for the radical anions of **1-5**

Radical species	Isotropic coupling	g and hyperfine tensors	Phosphorus spin densities
$[K(THF)_3]^+ \cdot \mathbf{1}^{\bullet-}$	g = 2.0062, a = 80.4 G	$g_{//}$ = 2.0045, $a_{//}(^{31}P)$ = 211 G; $g_{\perp}$ = 2.0087, $a_{\perp}(^{31}P)$ = 10.2 G	$\rho_s(P)$ = 1.62 % $\rho_p(P)$ = 51.09 %
$[Li(DME)_3]^+ \cdot 1^{\bullet-}$	g = 2.0062, a = 79.3 G	$g_{//}$ = 2.0038, $a_{//}(^{31}P)$ = 211.5 G; $g_{\perp}$ = 2.0091, $a_{\perp}(^{31}P)$ = 8.9 G	$\rho_s(P)$ = 1.60 % $\rho_p(P)$ = 51.37 %
$\mathbf{2}^{\bullet-}$, Ref.S2	g = 2.005, a = 54.1 G	$g_{//}$ = 2.003, $a_{//}(^{31}P)$ = 162 G; $g_{\perp}$ = 2.006, $a_{\perp}(^{31}P)$ = 2.20 G	$\rho_s(P)$ = 1.17 % $\rho_p(P)$ = 40.7 %
$\mathbf{3}^{\bullet-}$, Ref.S3	g = 2.0049, a = 77.6 G	$g_{//}$ = 1.9986, $a_{//}(^{31}P)$ = 215 G; $g_{\perp}$ = 2.0075, $a_{\perp}(^{31}P)$ = 10.5 G	$\rho_s(P)$ = 1.60 % $\rho_p(P)$ = 52.0 %
$\mathbf{4}^{\bullet-}$, Ref.S4	g = 2.0039, a = 89.7 G	$g_{//}$ = 2.0018, $a_{//}(^{31}P)$ = 249 G; $g_{\perp}$ = 2.005, $a_{\perp}(^{31}P)$ = 9.97 G	$\rho_s(P)$ = 1.90 % $\rho_p(P)$ = 61.0 %
$\mathbf{5}^{\bullet-}$, Ref.S4	g = 2.0059, a = 78.7 G	$g_{//}$ = 2.0030, $a_{//}(^{31}P)$ = 217 G; $g_{\perp}$ = 2.0104, $a_{\perp}(^{31}P)$ = 7.83 G	$\rho_s(P)$ = 1.60 % $\rho_p(P)$ = 53.0 %



2 **3**



4 **5**

S2. Geoffroy, M.; Jouaiti, A.; Terron, G.; Cattani-Lorente, M. *J. Phys. Chem*. **1992**, *96*, 8241.

S3. Gouverd, C.; Brynda, M.; Berclaz, T.; Geoffroy, M. *J. Organomet. Chem*. **2006**, *691*, 72.

S4. Badri, A. A.; Chentit, M.; Geoffroy, M.; Jouaiti, A. *J. Chem. Soc., Fara. Trans*. **1997**, *93*, 3631.

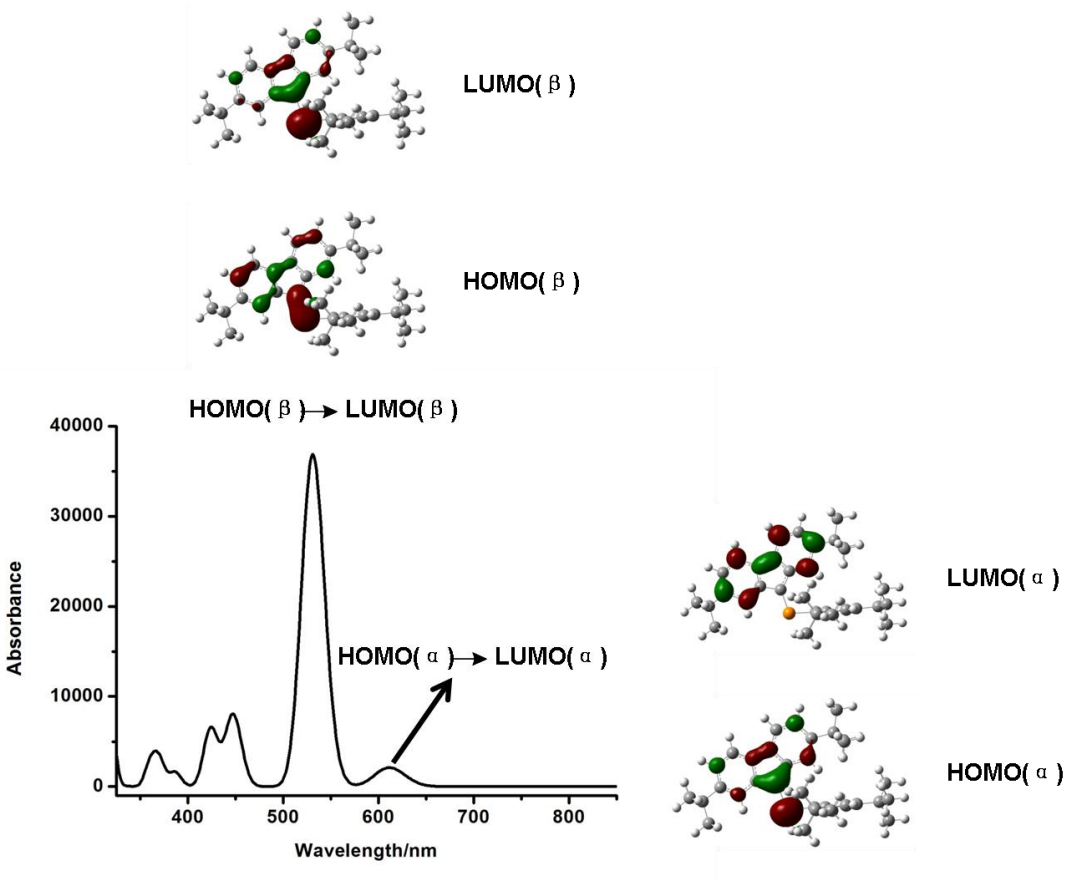


Figure S3. Calculated absorption spectrum of $\mathbf{1}^{\bullet-}$.

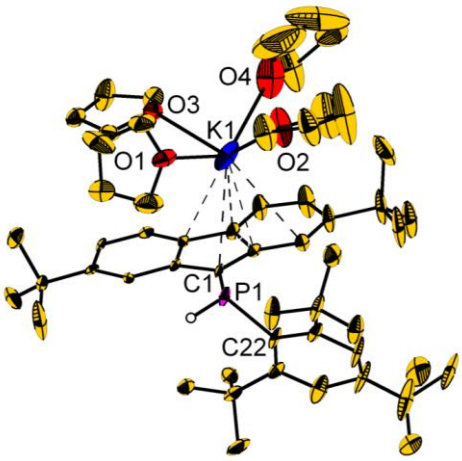


Figure S4. Thermal ellipsoid (50%) drawing of $[K(THF)_4]^+ \cdot [\mathbf{1H}]^-$. Except for H1, all other H atoms have been omitted for clarity.

Table S5. Experimental and Calculated Structural Parameters for Anion [**1H**]$^-$

	$[K(THF)_4]^+ \cdot [\mathbf{1H}]^-$	[**1H**]$^-$(Calculated)
P1–C1 (Å)	1.766(11)	1.788
P1–C22 (Å)	1.873(11)	1.904
∠C–P–C (^{o})	104.9(5)	107.7

Computational details

All the geometry optimizations were carried out at the (U)PBE0/6-31G(d) level of theory. The obtained stationary points were characterized by frequency calculations. The molecular orbitals and spin densities were calculated at the level of (U)PBE0/6-31G(d) at the optimized geometries. The UV-vis absorption spectrum was calculated using time-dependent DFT (TD-DFT) method and polarized continuum model (PCM) was adopted to consider solvent (THF) effects. All calculations were performed with the Gaussian 09 program suite.

Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kieth, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J., Gaussian, Inc., Wallingford CT, 2010.

Coordinates for optimized geometries:

1

P	-0.87692800	-1.51017300	-0.00067000
C	-3.97941700	-0.55911800	-0.01704500
H	-3.78019900	-1.62593800	-0.03170400
C	-5.29441800	-0.08590200	-0.00813200
C	-5.49866500	1.30527700	0.01172200
H	-6.51350200	1.69458600	0.01989300
C	-4.44192000	2.20844200	0.02038400
H	-4.63887300	3.27769200	0.03496600
C	-1.51682600	3.74352800	0.02104000
H	-2.28983900	4.50804900	0.03672500
C	-0.17130900	4.11513500	0.01086000
H	0.06919200	5.17313100	0.01989700
C	0.85780700	3.16723400	-0.01271800
C	0.50919300	1.80691900	-0.02154400
H	1.28669200	1.05167000	-0.04077400
C	-1.44897200	0.08365400	-0.01167200
C	-3.14004000	1.72167200	0.00929900
C	-1.84693800	2.39868000	0.00952000
C	-0.82573500	1.41775300	-0.00833000
C	-2.90952500	0.33407200	-0.00809200
C	-6.50524700	-1.02269600	-0.02060900
C	-7.35347000	-0.77859500	1.23823600
H	-7.71728300	0.25296600	1.29099800
H	-6.77124800	-0.97450400	2.14551500
H	-8.22773600	-1.44113600	1.24348000
C	-7.35553500	-0.74152400	-1.27032600
H	-7.71987000	0.29098500	-1.29176800
H	-8.22942700	-1.40415900	-1.29398500
H	-6.77454500	-0.91001900	-2.18388600
C	-6.09952200	-2.49873600	-0.04287500
H	-6.99779000	-3.12639300	-0.05146700
H	-5.51251300	-2.77390100	0.84075200
H	-5.51416500	-2.74735300	-0.93541800
C	2.33747600	3.55965400	-0.04050000
C	2.97504100	3.02895800	-1.33518200
H	2.48223100	3.45740500	-2.21546400
H	2.90338600	1.93823800	-1.40474300
H	4.03800500	3.29812100	-1.37531000
C	2.54010700	5.07629700	0.00494500
H	2.08486400	5.57536200	-0.85819500
H	3.61177500	5.30456400	-0.01093200

H	2.12220000	5.51610100	0.91784800
C	3.05547700	2.94486700	1.17218300
H	2.62555600	3.31617600	2.10959000
H	4.12001000	3.21124700	1.15782500
H	2.98364100	1.85201800	1.17798400
C	0.97561700	-1.44400000	0.01722500
C	1.67907400	-1.43829100	1.25679400
C	3.07392200	-1.30883800	1.22321000
H	3.61197900	-1.27572500	2.15882200
C	3.80585600	-1.23274800	0.04620700
C	3.09656700	-1.34537800	-1.14674800
H	3.66233700	-1.34772700	-2.06902400
C	1.70753700	-1.47095900	-1.21049800
C	1.02606300	-1.59975200	2.65621500
C	0.15039000	-2.86352200	2.70618600
H	0.74002000	-3.75407700	2.46055800
H	-0.70007900	-2.82545500	2.01789500
H	-0.25849300	-2.99078600	3.71562400
C	2.07723700	-1.78895400	3.76444700
H	2.73542400	-2.64389100	3.57321400
H	1.55521600	-1.97909300	4.70839500
H	2.69448200	-0.89636500	3.91536700
C	0.20982000	-0.35893700	3.05727500
H	0.82727500	0.54457400	3.00369800
H	-0.14029000	-0.46917300	4.09101200
H	-0.66591300	-0.20512000	2.42612700
C	5.33102500	-1.10350400	0.02093500
C	5.93297800	-2.37066100	-0.60919300
H	5.58227400	-2.51898100	-1.63600200
H	5.66289500	-3.26132800	-0.03091500
H	7.02720800	-2.29919000	-0.63569000
C	5.92577600	-0.93532000	1.42182700
H	5.53103800	-0.04555400	1.92585400
H	7.01299200	-0.81977100	1.34753200
H	5.73185600	-1.80668400	2.05752800
C	5.73532200	0.12026300	-0.81637000
H	5.37299700	0.05105700	-1.84742600
H	6.82787500	0.20819400	-0.85359500
H	5.33355100	1.04225000	-0.38191300
C	1.08137000	-1.66296300	-2.61744100
C	0.27816100	-0.42791900	-3.05888600
H	-0.59706200	-0.24644400	-2.43402100
H	-0.07098900	-0.56604100	-4.08957800
H	0.90436900	0.47081000	-3.03146700

C	0.20115400	-2.92398700	-2.65609800
H	0.77966400	-3.81025000	-2.37160100
H	-0.18240900	-3.07650800	-3.67194000
H	-0.66651600	-2.86351800	-1.99136300
C	2.15310900	-1.88035600	-3.70019500
H	2.80150000	-2.73552100	-3.47859700
H	2.77921800	-0.99467600	-3.85561400
H	1.64967600	-2.08580300	-4.65096700

1$^{\bullet-}$

P	-0.88427800	-1.56613900	-0.01810500
C	-1.48350400	0.09427000	-0.01289100
C	-0.87397600	1.40333200	-0.00345100
C	-1.89967800	2.40641200	0.01228000
C	-3.17347200	1.73158900	0.00910800
C	-2.91229600	0.33041400	-0.00746100
C	-3.99424000	-0.56863700	-0.01539100
H	-3.78187500	-1.63363600	-0.02817000
C	-5.30682800	-0.10760300	-0.00774300
C	-5.53854500	1.28788700	0.00993400
H	-6.55948300	1.66495600	0.01681900
C	-4.48814900	2.19494700	0.01831300
H	-4.69559300	3.26448700	0.03174000
C	-1.56069000	3.75485700	0.02617000
H	-2.33954000	4.51673100	0.03971400
C	-0.22263800	4.13732400	0.02224400
H	0.01659400	5.19638000	0.03352900
C	0.80711300	3.17559900	0.00261800
C	0.46715100	1.82149900	-0.00972700
H	1.25183800	1.07194000	-0.02685200
C	2.28927300	3.57041500	-0.01943900
C	3.01160900	2.95482400	1.19010400
H	2.57615400	3.32125200	2.12728600
H	4.07825400	3.22127900	1.18079400
H	2.93496000	1.86274000	1.19134500
C	2.93789900	3.04985900	-1.31255000
H	4.00278500	3.31992700	-1.35092800
H	2.44329700	3.48064000	-2.19115700
H	2.86165700	1.96014500	-1.38626900
C	2.49433300	5.08709100	0.03338000
H	2.06727600	5.52060200	0.94526200

H	2.03722200	5.58761100	-0.82814300
H	3.56712100	5.31797700	0.02283500
C	-6.50894600	-1.05759600	-0.01916100
C	-6.09282800	-2.53069200	-0.03891400
H	-5.49814400	-2.79335000	0.84292900
H	-5.49960200	-2.76980500	-0.92840000
H	-6.98524800	-3.16962400	-0.04671900
C	-7.36544400	-0.79152900	-1.26800500
H	-6.77933000	-0.95997300	-2.17852400
H	-7.72884400	0.24126200	-1.29445600
H	-8.23853100	-1.45846800	-1.29183000
C	-7.36407900	-0.82455400	1.23714600
H	-8.23765200	-1.49123600	1.24392200
H	-7.72679400	0.20737600	1.29157500
H	-6.77732000	-1.01769800	2.14232900
C	0.98726900	-1.45524600	0.00776300
C	1.73941100	-1.46053700	-1.21216900
C	3.12968800	-1.33224900	-1.14804900
H	3.69764700	-1.31317400	-2.06964300
C	3.83711400	-1.22786400	0.04555700
C	3.10105000	-1.31358700	1.21828800
H	3.63525700	-1.27320000	2.15625100
C	1.70502700	-1.44834000	1.24300800
C	1.05856600	-1.61631300	2.64596700
C	0.31470600	-2.96102200	2.72881200
H	-0.11141300	-3.08838600	3.73302700
H	1.00398500	-3.79416300	2.54195700
H	-0.50110700	-3.01259800	2.00264500
C	2.10332200	-1.65353500	3.77585100
H	2.65612000	-0.71082400	3.86689100
H	2.82370500	-2.47271700	3.66032800
H	1.57743700	-1.81221800	4.72461300
C	0.11670100	-0.45213000	2.99390100
H	-0.25733100	-0.57800400	4.01917100
H	-0.73953500	-0.39242600	2.32150400
H	0.65032200	0.50391200	2.93984800
C	5.36128400	-1.08027800	0.02320800
C	5.95471400	-0.92573100	1.42636100
H	5.76144300	-1.80580700	2.05039100
H	5.54906900	-0.04659900	1.93981400
H	7.04239600	-0.80117200	1.35630500
C	5.98413600	-2.32794900	-0.62453900
H	7.07851900	-2.24120300	-0.65651400
H	5.62670500	-2.46856700	-1.65010400

H	5.72757800	-3.22925100	-0.05605600
C	5.75316000	0.16123700	-0.79358600
H	6.84555000	0.26800400	-0.82815700
H	5.33226900	1.06893600	-0.34763200
H	5.38976300	0.10091300	-1.82471800
C	1.12681300	-1.63317600	-2.62881800
C	2.19794100	-1.67555800	-3.73298500
H	2.91096600	-2.49853200	-3.59979500
H	2.75745800	-0.73553600	-3.81037600
H	1.69483700	-1.83182800	-4.69437100
C	0.38189100	-2.97640600	-2.72528400
H	-0.45190300	-3.02388400	-2.01958000
H	1.06466800	-3.81022100	-2.51868000
H	-0.01947000	-3.10636400	-3.73931600
C	0.19645200	-0.46688200	-3.00076200
H	-0.16580500	-0.60105500	-4.02918400
H	0.73577100	0.48626700	-2.95048900
H	-0.66779000	-0.39457600	-2.33972100

[**1H**]$^{-}$

C	0.708541	1.582413	0.383910
C	-0.620287	2.013898	0.582531
C	1.276211	3.810560	-0.454850
C	-0.034213	4.208450	-0.243053
C	-1.000663	3.316063	0.287115
C	2.712345	0.478472	0.266383
C	2.927917	1.819535	-0.210597
C	1.671556	2.507443	-0.141402
C	4.206036	2.217114	-0.606999
C	5.091320	0.012811	-0.042059
C	3.822854	-0.391575	0.353651
C	5.269241	1.331000	-0.531021
C	6.308576	-0.914458	0.043579
C	-3.339751	2.754675	1.126381
C	-2.431358	3.819159	0.504716
C	7.364965	-0.297360	0.975050
C	6.918157	-1.098187	-1.356072
C	-2.418374	5.032666	1.449016
C	5.957271	-2.301898	0.586740
C	-3.041481	4.237380	-0.843122
C	-0.994687	-1.565149	-0.986689

C	-2.143712	-1.780803	1.155851
C	-3.360334	-1.608830	0.485759
C	-3.437837	-1.312825	-0.870604
C	-2.243300	-1.348328	-1.579078
C	-4.757707	-1.036422	-1.594720
C	-4.670482	0.307593	-2.334804
C	-5.947071	-0.969476	-0.632314
C	-5.028002	-2.156126	-2.613212
C	-2.236265	-2.173830	2.655510
C	-2.113147	-0.950711	3.581296
C	-3.593475	-2.831354	2.976226
C	-1.179526	-3.231700	3.015275
C	0.154433	-1.785323	-2.003589
C	0.513025	-0.469595	-2.711206
C	1.426270	-2.399697	-1.415307
C	-0.325468	-2.806176	-3.062035
C	1.333543	0.318325	0.605339
P	0.557537	-1.034150	1.480684
C	-0.918764	-1.627490	0.435372
H	-4.351362	3.159876	1.259972
H	-3.411978	1.863023	0.493684
H	-2.970302	2.437258	2.108232
H	7.687930	0.686857	0.620074
H	6.957191	-0.167652	1.984007
H	8.252074	-0.942854	1.041572
H	7.220646	-0.140001	-1.791161
H	6.188750	-1.554396	-2.035019
H	7.804059	-1.747311	-1.314459
H	-3.437425	5.411834	1.609265
H	-1.996931	4.756516	2.422278
H	-1.812921	5.851530	1.046563
H	5.219280	-2.806623	-0.046835
H	6.857993	-2.928375	0.620941
H	5.549257	-2.245315	1.602202
H	-4.064293	4.616874	-0.709263
H	-3.077543	3.383155	-1.529032
H	-2.448648	5.022501	-1.324620
H	-5.603460	0.506497	-2.878591
H	-3.850493	0.318808	-3.059845
H	-4.501146	1.130923	-1.632373
H	-6.860870	-0.729656	-1.189598
H	-6.112764	-1.925100	-0.121447
H	-5.804789	-0.194418	0.129467
H	-5.967979	-1.971297	-3.150162

H	-5.104674	-3.127617	-2.111386
H	-4.224526	-2.226776	-3.354039
H	-2.258768	-1.256775	4.626692
H	-2.883415	-0.209561	3.335115
H	-1.133333	-0.478004	3.488673
H	-3.824997	-3.651835	2.286742
H	-3.553473	-3.243538	3.991704
H	-4.426659	-2.119996	2.959017
H	-1.333103	-3.573314	4.047571
H	-1.260518	-4.101369	2.352339
H	-0.163921	-2.835131	2.949702
H	-0.355386	-0.047447	-3.231440
H	1.299823	-0.646321	-3.456347
H	0.876150	0.270021	-1.993251
H	1.198889	-3.272382	-0.791923
H	2.072689	-2.732222	-2.237723
H	1.993329	-1.677335	-0.833405
H	-0.620824	-3.750992	-2.589750
H	0.496991	-3.016401	-3.756994
H	-1.169473	-2.453783	-3.662045
H	1.997516	4.520465	-0.859705
H	-0.322338	5.228016	-0.492376
H	6.257577	1.663355	-0.842698
H	4.373509	3.230601	-0.971637
H	3.672604	-1.392326	0.749996
H	-2.280028	-1.202381	-2.654653
H	-1.344397	1.304884	0.974478
H	-4.280123	-1.687295	1.049076
H	1.515422	-2.056400	1.240326

$[K(THF)_3]^+ \cdot \mathbf{1}^{\bullet-}$

K	1.810209	1.379262	0.211328
P	-0.54587	-2.11259	0.727266
O	0.970801	3.941267	0.415757
O	4.413595	1.994813	-0.2594
O	2.722448	0.567176	2.649928
C	0.187762	-1.17862	-0.58712
C	-0.26439	-0.12538	-1.46715
C	0.785338	0.212145	-2.39023
C	1.908933	-0.6476	-2.10884
C	1.53908	-1.48603	-1.01239
C	2.460909	-2.44495	-0.54161

H	2.157935	-3.09805	0.271511
C	3.713698	-2.5848	-1.12815
C	4.056329	-1.73457	-2.20987
H	5.023022	-1.84626	-2.69582
C	3.171821	-0.78241	-2.69366
H	3.45424	-0.16321	-3.54441
C	0.598489	1.237693	-3.31738
H	1.388569	1.49364	-4.02243
C	-0.61109	1.92256	-3.36068
H	-0.73959	2.7023	-4.10443
C	-1.6675	1.600455	-2.48014
C	-1.47717	0.584569	-1.54359
H	-2.28346	0.315241	-0.86919
C	-3.02732	2.306043	-2.54933
C	-4.10119	1.284952	-2.96143
H	-3.86958	0.8548	-3.94247
H	-5.08624	1.766503	-3.02449
H	-4.16895	0.461614	-2.24238
C	-3.38923	2.889203	-1.1741
H	-4.36339	3.393216	-1.21538
H	-2.64036	3.624999	-0.85495
H	-3.44818	2.112833	-0.40475
C	-3.04525	3.451268	-3.5659
H	-2.857	3.095861	-4.58512
H	-2.29905	4.219425	-3.32844
H	-4.03015	3.932634	-3.56171
C	4.718266	-3.64897	-0.67385
C	4.19624	-4.48602	0.49685
H	3.280422	-5.02559	0.232776
H	3.984225	-3.8669	1.37653
H	4.94976	-5.22814	0.785441
C	6.028192	-2.97846	-0.22923
H	5.855686	-2.32237	0.632962
H	6.468268	-2.37424	-1.03011
H	6.767641	-3.7344	0.064084
C	5.013789	-4.60299	-1.84336
H	5.733719	-5.37287	-1.53813
H	5.434045	-4.07289	-2.70426
H	4.097318	-5.1027	-2.17551
C	-2.36245	-1.66496	0.748323
C	-2.87308	-0.69182	1.666107
C	-4.21991	-0.33108	1.588603
H	-4.60424	0.416013	2.271016
C	-5.10986	-0.89059	0.676447

C	-4.61707	-1.90237	-0.13537
H	-5.30373	-2.3853	-0.81427
C	-3.28429	-2.33851	-0.10965
C	-2.9512	-3.5794	-0.98384
C	-2.40403	-4.71327	-0.09793
H	-2.21075	-5.60152	-0.71253
H	-3.134	-4.98543	0.673774
H	-1.46832	-4.43544	0.394569
C	-4.20097	-4.1632	-1.6686
H	-4.64094	-3.47552	-2.40041
H	-4.97628	-4.45712	-0.9515
H	-3.90293	-5.06495	-2.21481
C	-1.96863	-3.26052	-2.12261
H	-1.86062	-4.143	-2.76612
H	-0.97894	-2.98307	-1.76052
H	-2.3438	-2.43562	-2.73917
C	-6.57251	-0.43799	0.651586
C	-7.37324	-1.1144	-0.46476
H	-7.42342	-2.20104	-0.3325
H	-6.94448	-0.90817	-1.45224
H	-8.40174	-0.73517	-0.46181
C	-7.23123	-0.78842	1.996298
H	-8.28176	-0.47136	2.00201
H	-6.72703	-0.29483	2.834125
H	-7.19888	-1.86875	2.176592
C	-6.64847	1.081367	0.43339
H	-7.69416	1.41326	0.439412
H	-6.20696	1.360679	-0.52951
H	-6.11974	1.634969	1.216522
C	-2.04207	-0.02484	2.793406
C	-2.87641	0.922746	3.670939
H	-3.70777	0.410091	4.167331
H	-3.27638	1.773673	3.107088
H	-2.22904	1.328816	4.457083
C	-1.48989	-1.09998	3.745348
H	-0.82869	-1.80201	3.23039
H	-2.31226	-1.66813	4.195009
H	-0.92235	-0.62563	4.55783
C	-0.90214	0.831219	2.221213
H	-0.34565	1.312616	3.037382
H	-1.30143	1.61253	1.56226
H	-0.21124	0.209039	1.648306
C	0.653027	4.708544	-0.75296
H	0.164241	4.049163	-1.47773

H	1.586738	5.086075	-1.19482
C	-0.22666	5.852885	-0.26958
H	-0.16914	6.730794	-0.9193
H	-1.27424	5.534292	-0.21718
C	0.327434	6.09484	1.133058
H	1.252406	6.681143	1.0815
H	-0.3702	6.614423	1.796018
C	0.62297	4.673096	1.593259
H	1.456063	4.609921	2.302433
H	-0.26084	4.210227	2.054104
C	2.977596	1.286359	3.855126
H	2.042771	1.744416	4.211956
H	3.692956	2.08777	3.637827
C	3.496286	0.260028	4.852967
H	3.320139	0.555004	5.891475
H	4.573686	0.106801	4.717948
C	2.723179	-0.98721	4.429259
H	3.186592	-1.92157	4.758095
H	1.700959	-0.95673	4.823585
C	2.708879	-0.84653	2.913422
H	3.602365	-1.29386	2.456532
H	1.822058	-1.28347	2.441343
C	4.987826	2.478393	-1.47719
H	4.236784	2.41565	-2.27302
H	5.262229	3.533692	-1.34016
C	6.212428	1.610902	-1.74686
H	6.98989	2.141628	-2.30396
H	5.922938	0.718659	-2.31252
C	6.631318	1.212958	-0.33291
H	7.182177	2.028061	0.151892
H	7.249346	0.311	-0.30131
C	5.276835	1.013402	0.327989
H	4.882982	0.010094	0.115233
H	5.278707	1.170029	1.411006