Two Phosphaalkene Radical Cations with Inverse Spin Density Distributions

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Contents

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**[S1] and **2**[S2] were synthesized according to literature methods. The ^{1}H NMR spectra were performed using a Bruker DRX-500 at variable-temperature in ppm downfield from Me_4Si. 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. All hydrogen atoms were found in different maps and refined using a riding model. CCDC-1049267 contains the supplementary crystallographic data for this paper.

Synthesis of $\mathbf{1}^{\bullet+}\cdot[Al(OR_F)_4]^-$:

Under anaerobic and anhydrous conditions, a mixture of **1** (0.113g, 0.300 mmol) and $Ag[Al(OR_F)_4]$ (0.321 g, 0.299 mmol) in CH_2Cl_2 (≈ 40 mL) was stirred at room temperature for 1 day. The resultant purple solution was filtered to remove the gray precipitate (Ag metal). The filtrate was then concentrated and stored at around -20 ^{o}C for 1 day to afford X-ray-quality crystals of phosphaalkene radical-cation salts. Yield: 0.193 g, 56.6 %; M.p.: 65-70 ^{o}C; UV-Vis (CH_2Cl_2): λ_{max} = 768, 550, and 375 nm; Elemental analysis calcd (%): C, 34.86； H, 3.08； N, 2.08; found: C 34.48, H 2.97; N 2.14.

Synthesis of 2a:

Under anaerobic and anhydrous conditions, a mixture of phosphaalkene **2** (0.167 g, 0.302 mmol) and $NO[Al(OR_F)_4]$ (0.301 g, 0.302 mmol) in CH_2Cl_2 (≈ 60 mL) was stirred at -50 ^{o}C for 2 hours. The resultant green solution was filtered and the filtrate was then concentrated and stored at around -20 ^{o}C for two weeks. In this process, the color gradually turns from green to yellow. Finally, the colorless crystals of **2a** were afforded from the yellow solution. Yield: 0.214 g, 46.9 %; m.p.: 208-212 ^{o}C; ^{1}H NMR (500 M Hz, CD_2Cl_2, 293 K) δ 7.99-6.50 (6H, m, fluorenyl), 7.71 (1H, s, Mes*), 7.27 (1H, s, Mes*), 8.38, 7.41 (1H, d, $^1J_{P\text{-}H}$ = 485 Hz, P*H*), 5.45, 5.42 (1H, d, $^2J_{P\text{-}H}$ = 14 Hz, P-C*H*), 1.86 (9H, s, -C(CH_3)$_3$), 1.47 (9H, s, -C(CH_3)$_3$), 1.43 (9H, s, -C(CH_3)$_3$), 1.38 (3H, s, -CH_3), 1.30 (3H, s, -CH_3), 1.03 (9H, s, -C(CH_3)$_3$). ^{31}P NMR (202 MHz, CD_2Cl_2, 293 K) δ 24.83. Elemental analysis calcd (%): C 43.43, H 3.58; found: C 43.24, H 3.58.

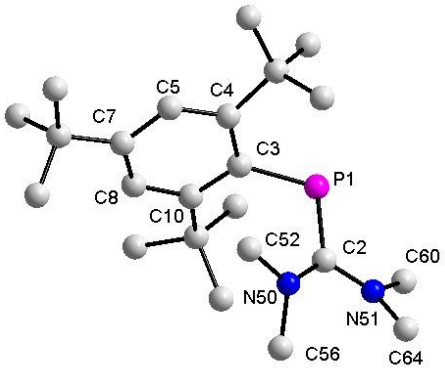
S1. P. Rosa, C. Gouverd, G. Bernardinelli, T. Berclaz and M. Geoffroy, *J. Phys. Chem. A*, 2003, **107**, 4883.

S2. A. Decken, C. Carmalt, J. A. C. Clyburne, and A.H. Cowley, *Inorg. Chem.*, 1997, **36**, 3741.

Table S1 Crystal data and structure refinement.

	$\mathbf{1}^{\bullet+}\cdot[Al(OR_F)_4]^-$
formula	$C_{79}H_{84}Al_2Cl_2F_{72}N_4O_8P_2$
Mr [g mol^{-1}]	2772.30
crystal system	Triclinic
space group	*P*-1
Z	2
μ (mm^{-1})	0.283
a (Å)	11.084(2)
b (Å)	20.020(4)
c (Å)	25.622(5)
α (°)	105.652(3)
β (°)	92.715(3)
γ (°)	97.800(3)
V [Å^3]	5402.7(17)
R1 (I>2σ(*I*))	0.0956
wR2 (all data)	0.2403

Table S2 Experimental and calculated structural parameters for phosphaalkene **1**[a] and **1**$^{\bullet+}$ species.



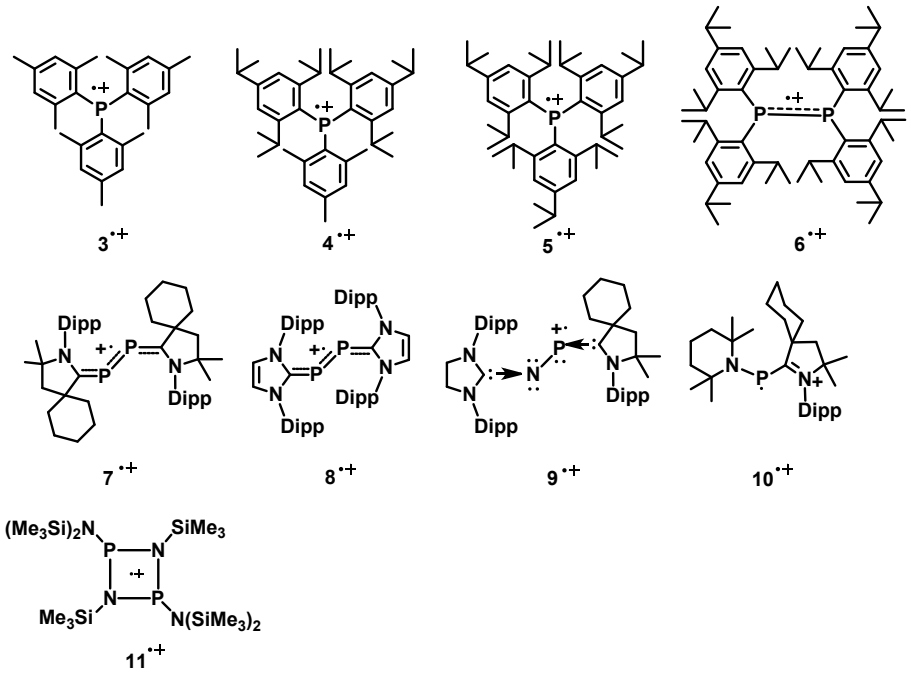
	Experimental		Calculated	
	1[a]	**1**$^{\bullet+}$[a]	$\mathbf{1}_{opt}$	$\mathbf{1}^{\bullet+}_{opt}$
P1-C2 (Å)	1.782	1.865(6)	1.741	1.860
P1-C3 (Å)	1.857	1.818(5)	1.863	1.820
C2-N51(Å)	1.362	1.326(7)	1.395	1.347
C2-N50 (Å)	1.372	1.331(7)	1.376	1.340
∠C3-P1-C2 (°)	105.4	103.8(2)	105.06	105.03
∠P1-C2-N51(°)	118.3	115.8(4)	116.87	114.08
∠P1-C2-N50 (°)	126.1	124.6(4)	130.77	127.64
∠N51-C2-N50 (°)	115.5	119.5(5)	112.36	118.23

[a] Structural parameters from the $[Cu\{Mes^*PC(NMe_2)_2\}_2]BF_4$ complex.[S3] The average bond lengths and angles were listed.

S3. L. Weber, J. Krümberg, H. –G. Stammler and B. Neumann, Z. *Anorg. Allg. Chem.*, 2006, **632**, 879.

Table S3 Hyperfine coupling cntansts and *g* values obtained for the phosphorus radical cations of **1**-**11**.

Radical cation species	*a* (G)	*g*	Measured tempreature (K)
1$^{\bullet+}$	101.6 G	2.0074	273 K
2$^{\bullet+}$	23.9 G	1.9008	273 K
3$^{\bullet+}$, Ref. S4	239 G	2.0056	298 K
4$^{\bullet+}$, Ref. S5	236 G	2.009	273 K
5$^{\bullet+}$, Ref. S5	233 G	2.008	273 K
6$^{\bullet+}$, Ref. S6	176 G	2.009	273 K
7$^{\bullet+}$, Ref. S7	42 G	2.009	298 K
8$^{\bullet+}$, Ref. S7	44 G	2.008	298 K
9$^{\bullet+}$, Ref. S8	44 G	2.008	298 K
10$^{\bullet+}$, Ref. S9	99 G	2.007	298 K
11$^{\bullet+}$, Ref. S10	263 and 224 G	2.0064	298 K



Mes*: 2,4,6-^{t}Bu$_3$C$_6$H$_2$; L: (3,5-Me$_2$C$_6$H$_3$)(Np)N, Np = neopentyl; Dipp: 2,6-^{i}Pr$_2$C$_6$H$_3$

S4. G. Ménard, J. A. Hatnean, H. J. Cowley, A. J. Lough and J. M. Rawson, *J. Am. Chem. Soc*., 2013, **135**, 6446.

S5. X. Pan, X. Chen, T. Li, Y. Li and X. Wang. *J. Am. Chem. Soc.*, 2013, **135**, 3414.

S6. X. Pan, Y. Su, X. Chen, Y.Zhao, Y. Li, J. Zuo, and X. Wang, *J. Am. Chem. Soc.*, 2013, **135**, 5561.

S7. O. Back, B. Donnadieu, P. Parameswaran, G. Frenking and G. Bertrand, *Nat. Chem.*, 2010, **2**, 369.

S8. R. Kinjo, B. Donnadieu and G. Bertrand, *Angew. Chem., Int. Ed.*, 2010, **49**, 5930.

S9. O. Back, M. A. Celik, G. Frenking, M. Melaimi, B. Donnadieu and G. Bertrand, *J. Am. Chem. Soc.*, 2010, **132**, 10262.

S10. Y. Su, X. Zheng, X. Wang, X. Zhang, Y. Sui and X. Wang, *J. Am. Chem. Soc*., 2014, **136**, 6251.

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 spectra were calculated using time-dependent DFT (TD-DFT) method at the UPBE0/6-31G(d) level, and polarized continuum model (PCM) was adopted to consider solvent (CH_2Cl_2) effects. The hyperfine constants $a(^{31}P)$ were calculated at the UM06-2X/6-31G(d) level. All calculations were performed with the Gaussian 09 program suite.[S11]

S11. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, Jr. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Kieth, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

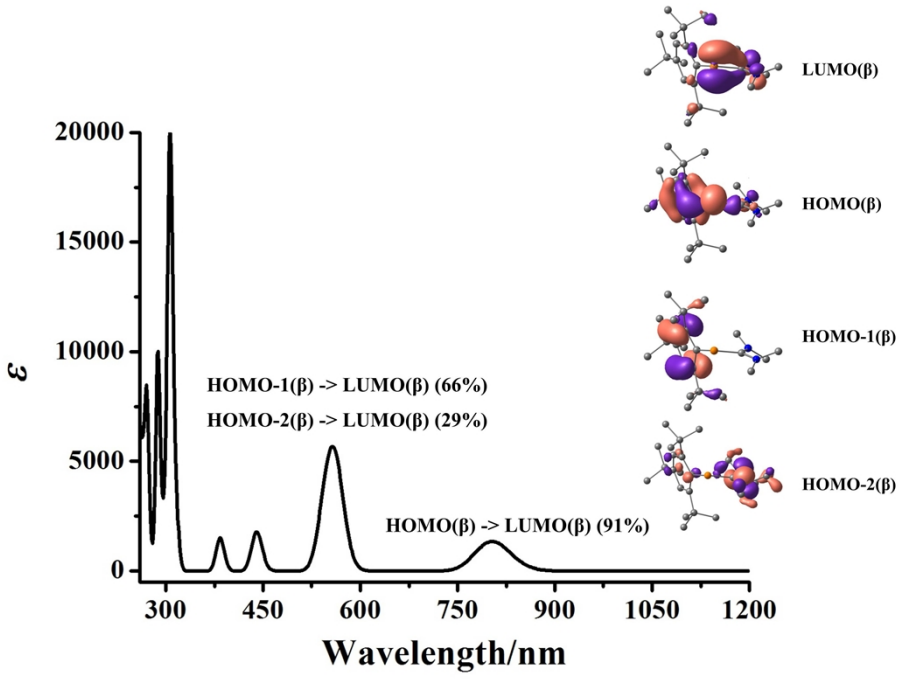


Fig. S1 Calculated absorption spectrum of $\mathbf{1}^{\bullet+}$.

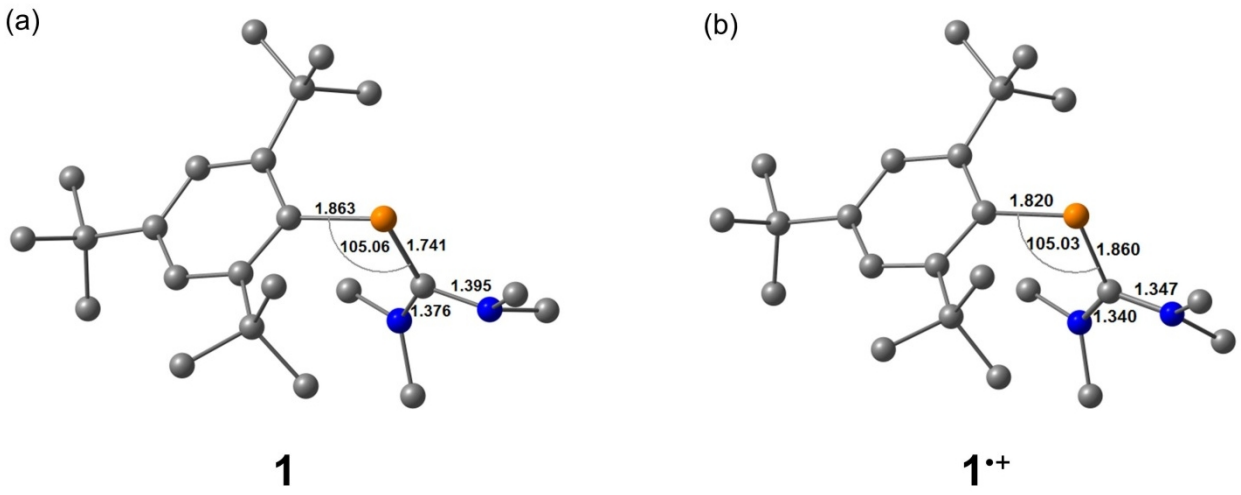


Fig. S2 Optimized geometry of (a) **1** and (b) **1**$^{\bullet+}$.

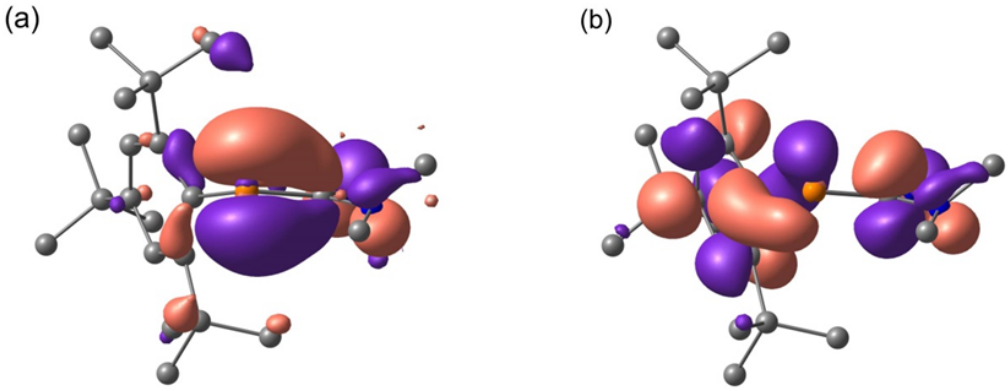


Fig. S3 HOMO (a) and LUMO (b) of **1**.

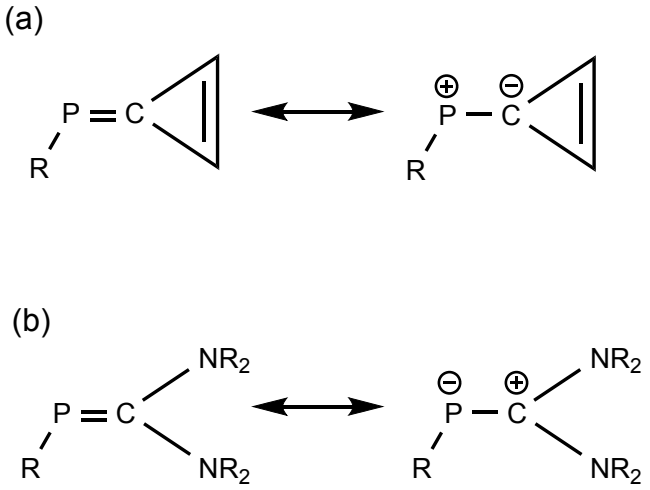


Fig. S4 (a) and (b) exhibit inverse electron density due to the polarization of P=C bond.

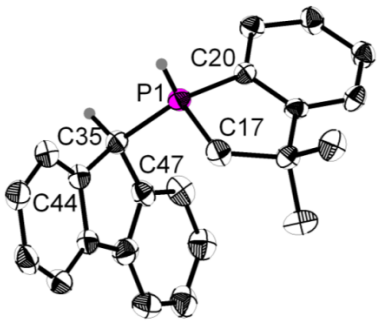


Fig. S5 Preliminary thermal ellipsoid (50%) drawing of **2a**. ^{t}Bu, the counterion $Al(OR_F)_4^-$ and all H atoms have been omitted for clarity (except for H1 and H35a). The structure could not be solved due to the highly disordered anion. Space group: *P*2(1)/c, Cell parameters: a = 14.7905(11) Å, b = 19.5329(14) Å, c = 23.2103(18) Å, α = 90.00 °, β = 97.935(2) °, γ = 90.00 °, V = 6641.3(9) Å^3.

Coordinates for calculated geometries:

1

P	1.830120000	0.622681000	-0.908130000
C	2.592899000	0.032360000	0.541281000
C	0.014277000	0.280473000	-0.673403000
C	-0.878105000	1.363553000	-0.420994000
C	-2.164109000	1.071508000	0.048450000
H	-2.825991000	1.889396000	0.294326000
C	-2.629379000	-0.225882000	0.224633000
C	-1.803959000	-1.254673000	-0.222848000
H	-2.195580000	-2.264098000	-0.192740000
C	-0.513447000	-1.046511000	-0.717690000
C	-0.544325000	2.858203000	-0.684943000
C	-0.010365000	3.027017000	-2.118852000
H	-0.734283000	2.642348000	-2.846256000
H	0.940395000	2.511264000	-2.274710000
H	0.152396000	4.091137000	-2.330748000
C	-1.798185000	3.746675000	-0.602662000
H	-2.591554000	3.407899000	-1.278364000
H	-1.523944000	4.765276000	-0.898761000
H	-2.206985000	3.808383000	0.412394000
C	0.454991000	3.445449000	0.326337000
H	0.057945000	3.380612000	1.347206000
H	0.620944000	4.507243000	0.103907000
H	1.421878000	2.938164000	0.292583000
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C	-4.868160000	-1.251420000	-0.251047000
H	-4.410071000	-2.185693000	-0.592507000
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H	-4.958825000	1.390436000	0.438909000
C	-3.836988000	-1.474018000	2.023956000
H	-3.340710000	-2.411736000	1.752716000
H	-4.814837000	-1.724941000	2.453437000
H	-3.236685000	-0.990649000	2.803356000
C	0.193385000	-2.266170000	-1.371613000
C	1.333670000	-2.846979000	-0.520769000
H	2.170813000	-2.155038000	-0.425832000
H	1.706672000	-3.768638000	-0.985817000
H	0.977191000	-3.101787000	0.484475000
C	0.715007000	-1.882278000	-2.767522000
H	-0.106614000	-1.531267000	-3.402373000

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H	-1.672291000	-3.116699000	-2.172778000
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N	2.058304000	-0.315589000	1.759946000
N	3.978858000	-0.118130000	0.507635000
C	0.809394000	0.208442000	2.257944000
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H	0.889360000	0.316140000	3.347883000
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H	2.925074000	-1.117092000	3.516036000
H	1.788328000	-2.185659000	2.666302000
H	3.407715000	-1.893451000	1.987129000
C	4.682459000	-0.160506000	-0.755180000
H	4.800332000	0.835449000	-1.209987000
H	5.680799000	-0.578660000	-0.578920000
H	4.145385000	-0.795996000	-1.462795000
C	4.763936000	0.512758000	1.556266000
H	4.158600000	0.642641000	2.453459000
H	5.636715000	-0.103714000	1.802606000
H	5.120466000	1.504179000	1.234342000

1$^{\bullet+}$

P	1.725019000	0.786944000	-0.891468000
C	2.598861000	0.073666000	0.587398000
C	-0.022506000	0.329368000	-0.672956000
C	-0.946240000	1.380112000	-0.386277000
C	-2.212301000	1.015855000	0.079903000
H	-2.910702000	1.796446000	0.344579000
C	-2.620965000	-0.307221000	0.216538000
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C	-0.647468000	2.885909000	-0.596318000
C	-0.164239000	3.122103000	-2.039111000
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H	0.795781000	2.644400000	-2.261495000
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H	1.859316000	-3.633494000	-1.050434000
H	1.101861000	-3.013228000	0.423881000
C	0.842883000	-1.701946000	-2.789319000
H	0.033226000	-1.336447000	-3.429387000
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H	-0.068642000	-4.098274000	-2.335864000
N	2.058111000	-0.304162000	1.754108000
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H	-0.019704000	-0.543790000	2.075250000
H	0.888181000	0.322172000	3.344482000
H	0.519759000	1.131746000	1.814574000
C	2.641627000	-1.366821000	2.567999000
H	3.116266000	-0.982898000	3.477131000
H	1.829575000	-2.039100000	2.862519000
H	3.366504000	-1.935410000	1.985251000
C	4.599048000	-0.055228000	-0.850969000
H	4.888508000	0.947339000	-1.185452000

H	5.500357000	-0.666968000	-0.748815000
H	3.958336000	-0.517307000	-1.602171000
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H	5.341443000	-0.728984000	1.881563000
H	5.626443000	0.901198000	1.237922000

2

P	-0.876928000	-1.510173000	-0.000670000
C	-3.979417000	-0.559118000	-0.017045000
H	-3.780199000	-1.625938000	-0.031704000
C	-5.294418000	-0.085902000	-0.008132000
C	-5.498665000	1.305277000	0.011722000
H	-6.513502000	1.694586000	0.019893000
C	-4.441920000	2.208442000	0.020384000
H	-4.638873000	3.277692000	0.034966000
C	-1.516826000	3.743528000	0.021040000
H	-2.289839000	4.508049000	0.036725000
C	-0.171309000	4.115135000	0.010860000
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C	0.857807000	3.167234000	-0.012718000
C	0.509193000	1.806919000	-0.021544000
H	1.286692000	1.051670000	-0.040774000
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C	-2.909525000	0.334072000	-0.008092000
C	-6.505247000	-1.022696000	-0.020609000
C	-7.353470000	-0.778595000	1.238236000
H	-7.717283000	0.252966000	1.290998000
H	-6.771248000	-0.974504000	2.145515000
H	-8.227736000	-1.441136000	1.243480000
C	-7.355535000	-0.741524000	-1.270326000
H	-7.719870000	0.290985000	-1.291768000
H	-8.229427000	-1.404159000	-1.293985000
H	-6.774545000	-0.910019000	-2.183886000
C	-6.099522000	-2.498736000	-0.042875000
H	-6.997790000	-3.126393000	-0.051467000
H	-5.512513000	-2.773901000	0.840752000
H	-5.514165000	-2.747353000	-0.935418000
C	2.337476000	3.559654000	-0.040500000

C	2.975041000	3.028958000	-1.335182000
H	2.482231000	3.457405000	-2.215464000
H	2.903386000	1.938238000	-1.404743000
H	4.038005000	3.298121000	-1.375310000
C	2.540107000	5.076297000	0.004945000
H	2.084864000	5.575362000	-0.858195000
H	3.611775000	5.304564000	-0.010932000
H	2.122200000	5.516101000	0.917848000
C	3.055477000	2.944867000	1.172183000
H	2.625556000	3.316176000	2.109590000
H	4.120010000	3.211247000	1.157825000
H	2.983641000	1.852018000	1.177984000
C	0.975617000	-1.444000000	0.017225000
C	1.679074000	-1.438291000	1.256794000
C	3.073922000	-1.308838000	1.223210000
H	3.611979000	-1.275725000	2.158822000
C	3.805856000	-1.232748000	0.046207000
C	3.096567000	-1.345378000	-1.146748000
H	3.662337000	-1.347727000	-2.069024000
C	1.707537000	-1.470959000	-1.210498000
C	1.026063000	-1.599752000	2.656215000
C	0.150390000	-2.863522000	2.706186000
H	0.740020000	-3.754077000	2.460558000
H	-0.700079000	-2.825455000	2.017895000
H	-0.258493000	-2.990786000	3.715624000
C	2.077237000	-1.788954000	3.764447000
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H	1.555216000	-1.979093000	4.708395000
H	2.694482000	-0.896365000	3.915367000
C	0.209820000	-0.358937000	3.057275000
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H	-0.665913000	-0.205120000	2.426127000
C	5.331025000	-1.103504000	0.020935000
C	5.932978000	-2.370661000	-0.609193000
H	5.582274000	-2.518981000	-1.636002000
H	5.662895000	-3.261328000	-0.030915000
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C	5.925776000	-0.935320000	1.421827000
H	5.531038000	-0.045554000	1.925854000
H	7.012992000	-0.819771000	1.347532000
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C	5.735322000	0.120263000	-0.816370000
H	5.372997000	0.051057000	-1.847426000
H	6.827875000	0.208194000	-0.853595000

H	5.333551000	1.042250000	-0.381913000
C	1.081370000	-1.662963000	-2.617441000
C	0.278161000	-0.427919000	-3.058886000
H	-0.597062000	-0.246444000	-2.434021000
H	-0.070989000	-0.566041000	-4.089578000
H	0.904369000	0.470810000	-3.031467000
C	0.201154000	-2.923987000	-2.656098000
H	0.779664000	-3.810250000	-2.371601000
H	-0.182409000	-3.076508000	-3.671940000
H	-0.666516000	-2.863518000	-1.991363000
C	2.153109000	-1.880356000	-3.700195000
H	2.801500000	-2.735521000	-3.478597000
H	2.779218000	-0.994676000	-3.855614000
H	1.649676000	-2.085803000	-4.650967000

2$^{\bullet+}$

P	-0.857936000	-1.554590000	-0.023015000
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C	-5.452336000	1.318181000	0.010524000
H	-6.470905000	1.692691000	0.017286000
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C	-1.524088000	3.745138000	0.017177000
H	-2.307683000	4.497514000	0.030722000
C	-0.192808000	4.123914000	0.004929000
H	0.050413000	5.179682000	0.009841000
C	0.844096000	3.170469000	-0.015896000
C	0.509032000	1.787646000	-0.018279000
H	1.298226000	1.045287000	-0.033108000
C	-1.432067000	0.051883000	-0.009559000
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C	-2.864489000	0.295649000	-0.006488000
C	-6.462724000	-1.013806000	-0.018647000
C	-7.304535000	-0.735590000	1.242090000
H	-7.658639000	0.299205000	1.290487000
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H	-8.183557000	-1.354944000	-1.289410000
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H	-6.999660000	-3.100920000	-0.043182000
H	-5.512817000	-2.785777000	0.852166000
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C	2.311154000	3.569934000	-0.047600000
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H	2.446458000	3.439536000	-2.228530000
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H	3.997352000	3.300048000	-1.382214000
C	2.511701000	5.086792000	-0.014563000
H	2.060482000	5.581416000	-0.881947000
H	3.582841000	5.310440000	-0.035369000
H	2.103078000	5.536067000	0.897545000
C	3.026296000	2.955289000	1.171118000
H	2.599437000	3.327984000	2.108681000
H	4.085511000	3.235318000	1.148341000
H	2.971809000	1.861645000	1.178783000
C	0.976299000	-1.469644000	0.010997000
C	1.663440000	-1.446797000	1.258706000
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H	3.585839000	-1.267299000	2.172750000
C	3.795244000	-1.218942000	0.058963000
C	3.094616000	-1.337902000	-1.140589000
H	3.665579000	-1.341645000	-2.059583000
C	1.709479000	-1.483004000	-1.216226000
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C	-0.009844000	-2.756288000	2.666482000
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H	-0.404816000	-2.892811000	3.679317000
C	2.023138000	-1.928971000	3.744262000
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H	1.488531000	-2.134562000	4.677248000
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C	0.304183000	-0.289668000	3.075105000
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H	-0.531822000	-0.022755000	2.423619000
C	5.319411000	-1.085975000	0.045130000
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H	5.587769000	-2.504392000	-1.610462000
H	5.650258000	-3.246025000	-0.003117000

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H	6.988798000	-0.795176000	1.383275000
H	5.710676000	-1.786434000	2.085535000
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H	5.370754000	0.066658000	-1.827514000
H	6.818061000	0.220789000	-0.826587000
H	5.328935000	1.061090000	-0.360518000
C	1.084351000	-1.672202000	-2.620921000
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H	1.010620000	0.461548000	-3.071860000
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H	0.653190000	-3.793278000	-2.317594000
H	-0.230567000	-3.045412000	-3.665489000
H	-0.750125000	-2.760184000	-2.015264000
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