Supporting Information

The 4,5,6-Triphospha[3]radialene Dianion: A Phosphorus Analogue of the Deltate Dianion. A NICS(0)$_{\pi zz}$ Examination of Their Aromaticity

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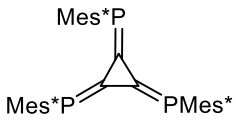
Contents



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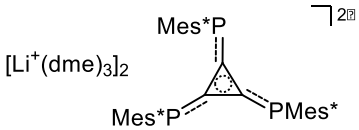
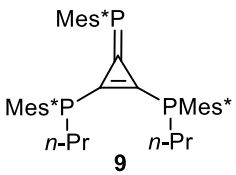


8^{2-}



9

1. General experimental procedures

All experiments were performed under an argon atmosphere unless otherwise noted. Dimethoxyethane (DME) and THF-d_8 used for the reactions or the spectroscopic measurements were dried by using a potassium mirror. The ^{1}H NMR (600 or 800 MHz) and ^{13}C NMR (150 or 201 MHz) spectra were measured with a BRUKER AVANCE III-600, or a BRUKER AVANCE III-800. Signals due to C_6D_5H (7.15 ppm) or THF-d_5 (3.58) in ^{1}H NMR and C_6D_6 (128.0 ppm) or THF-d_6 (25.2) in ^{13}C NMR spectra were used as internal references, respectively. ^{7}Li NMR (116 MHz) spectra were measured with a JEOL AL-300 spectrometer using LiCl in D_2O (0 ppm) as an external standard. The ^{31}P NMR (121 or 243 MHz) spectra were measured with a JEOL AL-300 or a BRUKER AVANCE III-600 spectrometer using 85% H_3PO_4 in water (0 ppm) as an external standard. UV-vis spectra were measured on a SHIMADZU UV-1700 PharmaSpec UV-vis spectrometer with a 1 mm quarts cell at ambient temperature. The electrochemical experiments were carried out on an ALS 1140A electrochemical analyzer using a glassy carbon disk working electrode, a Pt wire counter electrode, and Ag/0.01 M $AgNO_3$ reference electrode. The measurements were carried out in 1 mM THF solution containing 0.1 M (n-Bu)$_4$NPF$_6$ as a supporting electrolyte with scan rates of 50 mVs^{-1} at ambient temperature. Wet column chromatography was performed with Aluminiumoxid 90 active neutral (Merck®). All melting points were determined on a Yanaco micro melting point apparatus and were uncorrected. Elemental analyses were carried out at the Microanalytical Laboratory of the Institute for Chemical Research, Kyoto University.

2. Experimental procedure

2-1. Synthesis of dianionic compound $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$

To a suspension of **7** (87 mg, 0.10 mmol) in DME (1 mL) was added lithium metal (7 mg, 1 mmol) at room temperature. The reaction mixture was irradiated with ultrasonic waves for 5 hours. After removal of the residual lithium by decantation, the residual solution was recrystallized from DME/hexane at –30 ºC. Decantation of the resulting solid gave dianionic compound $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$ (115 mg, 81 μmol, 81%). $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$: brown crystals, m.p. 150-152 ˚C (decomp). ^{1}H NMR (800 MHz, THF-d_8) δ 1.26 (s, 27H), 1.70 (s, 54H), 3.27 (s, 36H), 3.43 (s, 24H), 7.19 (s, 6H); ^{7}Li NMR (116 MHz, THF-d_8) δ 1.4 (s); ^{13}C{^{1}H} NMR (201 MHz, THF-d_8) δ 32.3 (CH_3) 35.0 (CH_3), 40.2 (C), 58.9 (CH_3), 72.7 (CH_2), 120.3 (CH), 144.7 (C), 147.6 (m, C), 158.1 (m, C), 158.9 (C); ^{31}P NMR (121 MHz, C_6D_6) δ –51.2 (s). Anal. Calcd for $C_{81}H_{147}Li_2O_{12}P_3$: C, 68.52; H, 10.44%. Found: C, 68.06; H, 10.00%.

2-2. UV-vis monitoring of reaction of **7** with lithium

A solution of **7** (8.0 mg, 92 μmol) in DME (10 mL) was prepared in a reaction tube attached with a 1 mm quarts cell. Then, lithium powder (7 mg, 1 mmol) was added to the solution. The reaction mixture was stirred at room temperature and monitored by electronic spectroscopy. The UV-vis spectra are shown in Figure S1.

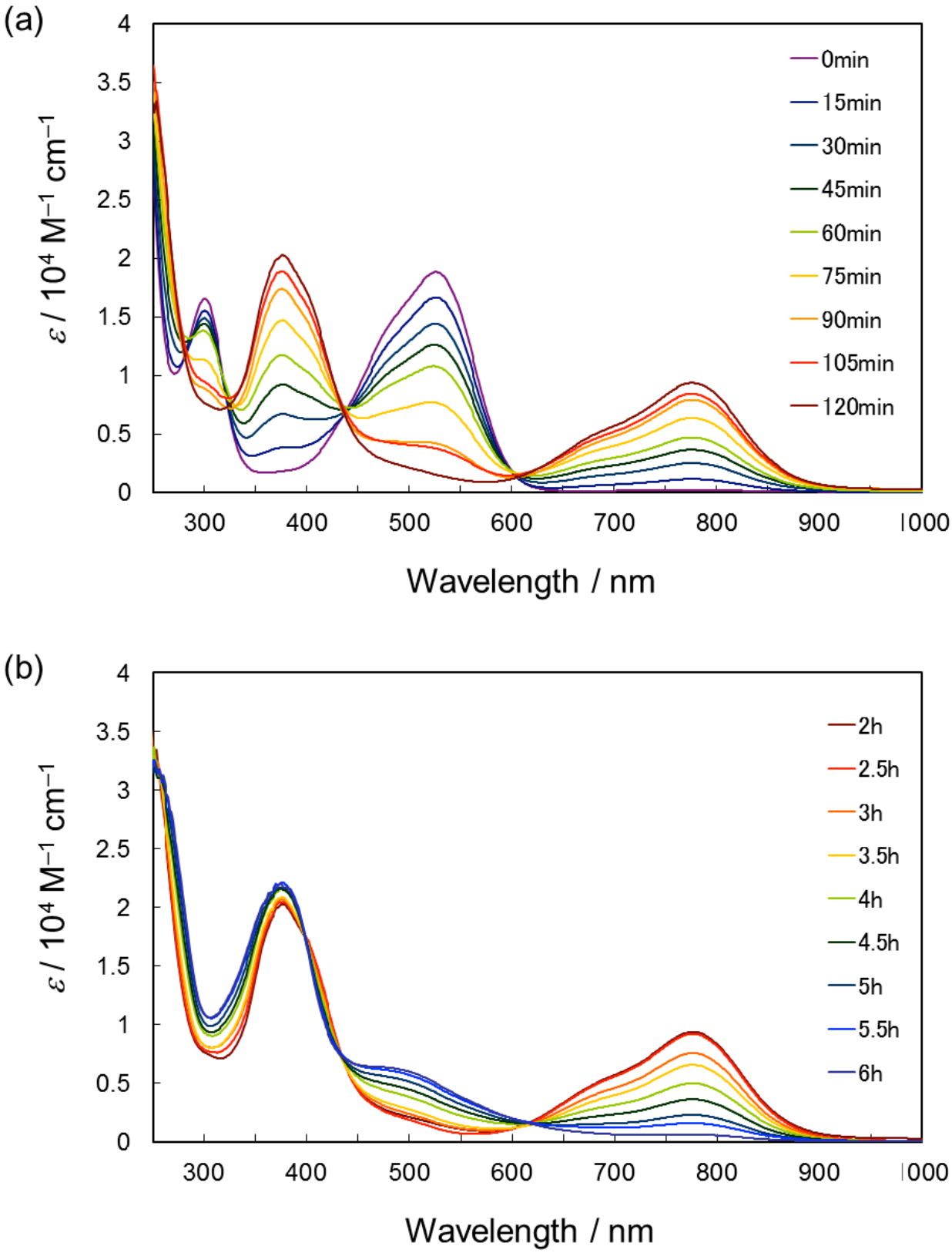


Figure. S1. UV-vis absorption spectra monitoring of the reaction of 7 with lithium (a) 0-2 h (b) 2-6 h.

2-3. Synthesis of 4-phosphatriafulvene **9**

To a solution of $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$ (43 mg, 30 μmol) in DME (1 mL) was added *n*-propyl bromide (27 μl, 0.30 mmol) at room temperature. The reaction mixture was stirred for 10 minutes. After the reaction mixture was stirred for 10 minutes, the solvent was removed under reduced pressure. Hexane was added to the residue, and then the mixture was filtered through Celite. After removal of the solvent, purification of the residue by alumina gel column chromatography (hexane) afforded 4-phosphatriafulvene **9** (27 mg, 28 μmol, 94%). **9**: orange crystals, m.p. 172-173 ºC (decomp), ^{1}H NMR (600 MHz, C_6D_6, 60 °C) δ 0.53 (t, J = 7.2 Hz, 3H), 0.63 (t, J = 7.5 Hz, 3H), 0.96-1.10 (m, 4H), 1.20 (s, 9H), 1.30 (s, 9H), 1.39 (s, 9H), 1.61 (s, 18H), 1.74 (s, 18H), 1.87 (s, 18H), 2.05-2.11 (br, 2H), 7.54 (d, J_{PH} = 2.4 Hz, 2H), 7.59 (d, J_{PH} = 2.4 Hz, 2H), 7.64 (d, J_{PH} = 1.8 Hz, 2H), one of the methylene protons was not assignable due to the overlap with those of the *t*-Bu groups. ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 60 °C) δ 15.0 (d, J_{PC} = 16 Hz, CH_3), 15.1 (d, J_{PC} = 13 Hz, CH_3), 20.0 (d, J_{PC} = 27 Hz, CH_2), 20.5 (d, J_{PC} = 27 Hz, CH_2), 31.0 (d, J_{PC} = 15 Hz, CH_2), 31.2 (CH_3), 31.3 (CH_3), 31.8 (CH_2), 32.3 (d, J_{PC} = 15 Hz, CH_2), 33.9 (d, J_{PC} = 9 Hz, CH_3), 34.3 (br, CH_3), 34.5 (d, J_{PC} = 8 Hz, CH_2), 34.97 (C), 35.00 (C), 35.2 (C), 39.2 (C), 39.7 (C), 30.8 (C), 121.7 (CH), 123.9 (br, CH), 126.2 (d, J_{PC} = 24 Hz, C), 126.4 (d, J_{PC} = 36 Hz, C), 140.4 (d, J_{PC} = 64 Hz, C), 148.4 (C), 141.6 (d, J_{PC} = 2 Hz, C), 151.8 (d, J_{PC} = 3 Hz, C), 151.9-152.5 (m, C), 155.4-156.1 (m, C), 156.5-156.8 (br, C), 159.0-160.3 (m, C); ^{31}P{^{1}H} NMR (243 MHz, C_6D_6) δ –29.9 to –27.7 (brs), –26.7 (d, J_{PP} = 22 Hz), 8.6 (d, J_{PP} = 5 Hz); HRMS (FAB), *m/z*: 950.7101 ([M^+]), calcd. for $C_{63}H_{101}P_3$: 950.7116; Anal. Calcd for $C_{63}H_{101}P_3$: C, 79.53; H, 10.70%. Found: C, 79.40; H, 10.73%.

3. X-Ray crystallographic analysis

Single crystals of $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$ and **9** were grown by slow recrystallization of its dimethoxyethane/hexane solution at –30° C and ether/ethanol solution at 0° C, respectively. Recrystallization of $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$ was under these conditions afforded single crystals of $[[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}\cdot 0.5(dme)]$. The intensity data were collected on a Rigaku Saturn70 CCD system with VariMax Mo Optic using Mo K_α radiation (λ = 0.71070 Å). The structure was solved by direct method (SIR-97[S1]) and refined by full-matrix least-squares procedures on F^2 for all reflections (SHELXL-97[S2]). All hydrogen atoms were placed using AFIX instructions, while all the other atoms were refined anisotropically. Cif files containing crystallographic data for $[[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}\cdot 0.5(dme)]$ and **9** have been deposited at the Cambridge Crystallographic Data Centre (CCDC-888281 and CCDC-888280). The data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. Packing structure of $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$ was shown in Figure S2. Molecular structure of **9** is shown in Figure S3. $[[Li(dme)_3]_2\cdot\mathbf{8}^{2-}\cdot 0.5(dme)]$: Formula $C_{83}H_{152}Li_2O_{13}P_3$, M_W = 1464.84; T = 103(2) K; monoclinic; space group $P2_1/c$ (#14); a = 12.6530(13) Å, b = 29.020(2) Å, c = 25.145(3) Å; β = 91.852(7); Z = 4; V =9228.0(16) Å^3; μ = 0.117 mm^{-1}; D_{calcd} = 1.054 Mg/m^3; $2\theta_{max}$ = 51.0°; 107878 measured reflections, 16949 independent reflections [R_{int} = 0.1648], 950 refined parameters; GOF = 1.010; R_1 ($I>2\sigma(I)$) = 0.0868; wR_2 (all data) = 0.2629; largest diff. peak and hole 0.718 and −0.515 e.Å^{-3}. **9**: Formula $C_{63}H_{101}P_3$, M_W = 951.35; T = 103(2) K; monoclinic; space group $P2_1/n$ (#14); a = 17.2445(3) Å, b = 10.5987(2) Å, c = 34.1242(7) Å; β = 101.0308(15); Z = 4; V = 6121.6(2) Å^3; μ = 0.132 mm^{-1}; D_{calcd} = 1.032

Mg/m^3; $2\theta_{max}$ = 51.0°; 52173 measured reflections, 11390 independent reflections [R_{int} = 0.0931], 624 refined parameters; GOF = 1.014; R_1 (I>2σ(I)) = 0.0522; wR_2 (all data) = 0.1446; largest diff. peak and hole 0.254 and −0.337 e.Å^{-3}.

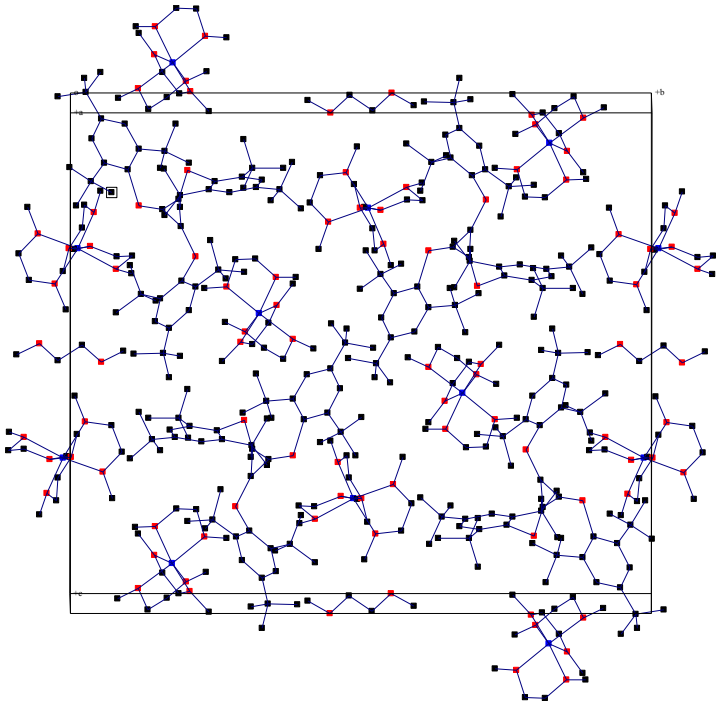


Figure. S2. Packing structure of $[Li^+(dme)_3]_2\cdot\mathbf{8}^{2-}$

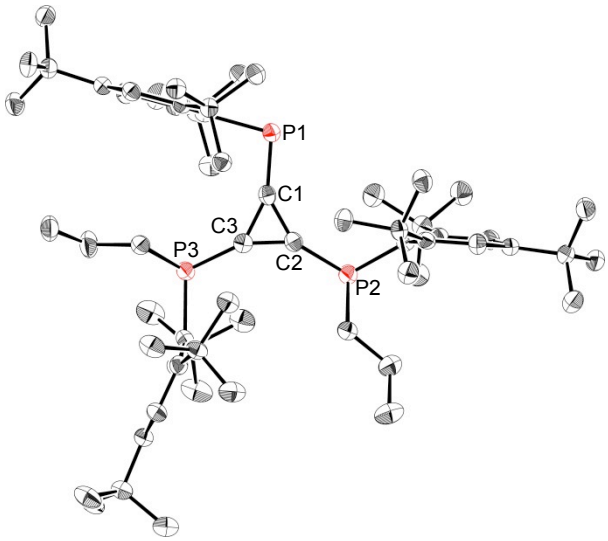


Figure. S3. Molecular structure of **9** with thermal ellipsoids set at 50% probability. Selected bond lengths (Å) and angles (°): P1–C1 = 1.677(3), P2–C2 = 1.777(3), P3–C3 = 1.769(3), C1–C2 = 1.437(4), C1–C3 = 1.444(4), C2–C3 = 1.356(4), C2–C1–C3 = 56.14(17), C3–C2–C1 = 62.20(19), C2–C3–C1 = 61.66(18).

4. Theoretical calculations

All theoretical calculations were carried out using the Gaussian 03 program.[S3] The geometries of **7'** and **8'**$^{2-}$ were optimized by using 6-31+G(3d) for P; 6-31G(d) for C and H basis sets with density function theory at the B3PW91 method. And the single point calculations were performed by using the same basis with Hartree-Fock method. The Cartesian coordinates in their optimized geometries are shown in Tables S1 and S2.

Table S1. Cartesian coordinates (Å) in optimized geometry of **7'**.

atom	X	Y	Z	atom	X	Y	Z
C	0.559695	-0.610643	0.039314	C	-0.335880	3.771711	-2.613821
C	-0.805619	-0.175713	0.033329	C	-0.262874	2.332985	-3.157152
C	0.253524	0.789048	0.040459	C	1.080107	4.363475	-2.462062
P	1.564772	-1.963488	0.038030	C	-1.020144	4.612476	-3.711657
P	-2.479906	-0.371211	0.025522	C	-0.657734	3.637883	2.632935
P	0.920957	2.337010	0.040946	C	0.800183	4.135862	2.678007
C	3.260545	-1.198487	0.014118	C	-0.743552	2.184169	3.131692
C	3.903934	-0.960761	-1.241190	C	-1.419010	4.498965	3.662780
C	5.052062	-0.158490	-1.244210	H	5.546214	0.077241	-2.178234
C	5.593995	0.345565	-0.073005	H	5.543611	0.317294	2.049244
C	5.050887	-0.022528	1.147007	H	4.227367	-1.948771	-4.580989
C	3.902565	-0.820110	1.234239	H	5.510765	-1.821904	-3.370194
C	3.460695	-1.577174	-2.596430	H	4.689383	-0.362608	-3.972931
C	4.544443	-1.408955	-3.681493	H	2.998253	-3.529803	-3.433792
C	3.248627	-3.098481	-2.456664	H	2.431683	-3.356224	-1.774516
C	2.190737	-0.904577	-3.149278	H	4.159985	-3.586289	-2.091297
C	3.457361	-1.269314	2.652614	H	2.342682	0.174955	-3.259772
C	4.567535	-1.031625	3.697891	H	1.323811	-1.059013	-2.504167
C	3.175291	-2.784166	2.687465	H	1.950792	-1.316297	-4.138130
C	2.226883	-0.483200	3.139751	H	4.747674	0.032464	3.886905
C	-2.666595	-2.221836	-0.015108	H	5.515451	-1.500045	3.409113
C	-2.676225	-2.973595	1.201101	H	4.254067	-1.473668	4.650380
C	-2.560452	-4.366607	1.107971	H	2.933571	-3.093731	3.711769
C	-2.498584	-5.014263	-0.114895	H	4.051861	-3.353199	2.355916
C	-2.649215	-4.286346	-1.284216	H	2.327341	-3.075838	2.057844
C	-2.768498	-2.890923	-1.275362	H	1.346465	-0.673986	2.524156
C	-2.861985	-2.369499	2.619688	H	2.426064	0.594110	3.124041
C	-4.035260	-1.369746	2.641684	H	1.983494	-0.769028	4.171224
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C	-3.224167	-3.453088	3.656650	H	-2.681085	-4.826951	-2.221644
C	-3.063857	-2.191874	-2.630935	H	-4.194548	-1.006340	3.664475
C	-1.839509	-1.427220	-3.166151	H	-4.961467	-1.846660	2.299995
C	-4.275204	-1.246221	-2.500585	H	-3.859500	-0.488897	2.014383
C	-3.449222	-3.209260	-3.725004	H	-1.294283	-0.834209	2.520266
C	-0.591963	3.419021	-0.004632	H	-0.738358	-2.405594	3.116931
C	-1.107368	3.849790	-1.267617	H	-1.713245	-1.350321	4.159123
C	-2.377830	4.438747	-1.287270	H	-3.458163	-2.963762	4.608900
C	-3.098124	4.660030	-0.124622	H	-2.396624	-4.144430	3.850805
C	-2.519667	4.382075	1.103050	H	-4.102733	-4.036083	3.357237
C	-1.254176	3.789997	1.207023	H	-2.062197	-1.013313	-4.158069

atom	X	Y	Z
H	-0.978644	-2.097825	-3.264741
H	-1.550054	-0.599121	-2.516485
H	-5.158263	-1.791221	-2.146701
H	-4.512415	-0.809535	-3.478692
H	-4.095760	-0.412737	-1.813302
H	-4.294352	-3.839730	-3.425802
H	-2.613494	-3.858233	-4.010071
H	-3.747194	-2.660419	-4.625548
H	-2.819789	4.742916	-2.227648
H	-3.070649	4.642429	1.997931
H	0.219099	2.330537	-4.143333
H	-1.268085	1.912136	-3.270412
H	0.309238	1.670351	-2.504939
H	1.588675	4.364104	-3.434157
H	1.710408	3.793127	-1.771633
H	1.033206	5.397444	-2.100504
H	-2.062197	-1.013313	-4.158069
H	-0.978644	-2.097825	-3.264741
H	-1.550054	-0.599121	-2.516485
H	-5.158263	-1.791221	-2.146701
H	-4.512415	-0.809535	-3.478692
H	-4.095760	-0.412737	-1.813302
H	-4.294352	-3.839730	-3.425802
H	-2.613494	-3.858233	-4.010071

atom	X	Y	Z
H	-2.819789	4.742916	-2.227648
H	-3.070649	4.642429	1.997931
H	0.219099	2.330537	-4.143333
H	-1.268085	1.912136	-3.270412
H	0.309238	1.670351	-2.504939
H	1.588675	4.364104	-3.434157
H	1.710408	3.793127	-1.771633
H	1.033206	5.397444	-2.100504
H	-1.158899	5.656594	-3.408663
H	-1.991993	4.203572	-4.010373
H	-0.384870	4.607661	-4.604600
H	1.178371	4.084381	3.706509
H	0.868698	5.176607	2.339998
H	1.477402	3.536712	2.059413
H	-0.385411	2.120787	4.167335
H	-0.138759	1.506294	2.527230
H	-1.779667	1.828581	3.108501
H	-2.438028	4.139199	3.843054
H	-1.468718	5.552615	3.364971
H	-0.891522	4.448179	4.622063
H	-4.091128	5.100234	-0.173257
H	-2.387136	-6.095080	-0.155203
H	6.474134	0.982959	-0.108927

Table S2. Cartesian coordinates (Å) in optimized geometry of **8'**$^{2-}$.

atom	X	Y	Z	atom	X	Y	Z
C	0.241808	0.778327	0.085081	H	-3.254336	4.698312	1.838424
C	0.557848	-0.594768	0.101022	H	-0.384104	4.470946	-4.700761
C	-0.789564	-0.182202	0.083073	H	-1.180042	5.603993	-3.595913
P	0.907487	2.392535	0.084612	H	-1.996271	4.098293	-4.087855
P	1.621736	-1.979183	0.131558	H	1.588710	4.371763	-3.474344
P	-2.521343	-0.405743	0.074171	H	1.644558	3.911072	-1.756787
C	-0.659253	3.454297	-0.039966	H	0.963155	5.490663	-2.238879
C	-1.132395	3.910587	-1.318080	H	-1.210653	1.871788	-3.230681
C	-2.383583	4.540666	-1.398972	H	0.343251	1.730937	-2.390145
C	-3.158292	4.777537	-0.276197	H	0.296566	2.279163	-4.086839
C	-2.649844	4.459485	0.971217	H	-2.825026	3.900910	3.666403
C	-1.401247	3.838349	1.128894	H	-1.955183	5.434301	3.404826
C	-0.342411	3.786673	-2.654462	H	-1.380749	4.270176	4.610265
C	-1.029072	4.538646	-3.815083	H	0.815163	4.212334	3.810724
C	1.052566	4.430852	-2.515532	H	0.423677	5.397707	2.541431
C	-0.218083	2.322604	-3.114966	H	1.214050	3.853448	2.113527
C	-0.906486	3.662969	2.594898	H	-0.114974	1.635058	2.437131
C	-1.831417	4.363396	3.613720	H	-1.828933	1.703875	2.860468
C	0.476272	4.323957	2.770214	H	-0.597482	2.108910	4.084998
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C	3.994642	-0.681641	1.224194	H	3.154104	-2.747754	3.918992
C	5.159590	0.088763	1.086741	H	4.419176	-3.008366	2.693411
C	5.727136	0.345750	-0.149344	H	2.699603	-2.952090	2.210409
C	5.170585	-0.231027	-1.278499	H	1.400868	-0.715059	2.463555
C	3.998774	-1.000392	-1.217805	H	2.279720	0.762251	2.871175
C	3.553740	-0.999536	2.683223	H	2.007842	-0.480254	4.121622
C	3.450009	-2.525839	2.882996	H	4.253577	-0.846268	4.718401
C	2.225477	-0.317036	3.055115	H	4.663624	0.578597	3.761546
C	4.584762	-0.515221	3.725687	H	5.585981	-0.932407	3.554621
C	3.537720	-1.650615	-2.555341	H	1.959061	-1.476807	-4.042520
C	2.226093	-1.030739	-3.072530	H	2.341332	0.050766	-3.211585
C	3.387232	-3.177040	-2.388363	H	1.409425	-1.199674	-2.368820
C	4.570791	-1.463268	-3.687251	H	4.338976	-3.626044	-2.071733
C	-2.667979	-2.296025	-0.003134	H	3.097650	-3.631218	-3.347703
C	-2.809496	-2.968051	-1.265423	H	2.616378	-3.412418	-1.648990
C	-2.733129	-4.368420	-1.306750	H	5.559323	-1.862831	-3.424592
C	-2.574863	-5.127701	-0.159906	H	4.687104	-0.413095	-3.983013
C	-2.573446	-4.494463	1.070954	H	4.217269	-2.008770	-4.571791
C	-2.653891	-3.098391	1.188630	H	-2.781563	-4.890641	-2.255213
C	-3.074288	-2.258785	-2.626144	H	-2.497889	-5.114023	1.956830
C	-1.853556	-1.446943	-3.096024	H	-2.053898	-1.008417	-4.085362
C	-4.321306	-1.355435	-2.528866	H	-0.971948	-2.093407	-3.178177
C	-3.381762	-3.260258	-3.760698	H	-1.623913	-0.644654	-2.393219
C	-2.769751	-2.541027	2.637730	H	-4.523676	-0.891267	-3.505588
C	-4.034594	-1.668023	2.769627	H	-4.166988	-0.559902	-1.794234
C	-1.519751	-1.747080	3.057143	H	-5.203355	-1.944606	-2.241559
C	-2.931113	-3.662820	3.686897	H	-4.236005	-3.909761	-3.527879
H	-2.782516	4.843575	-2.360150	H	-2.520767	-3.893082	-4.010223

atom	X	Y	Z
H	-3.634697	-2.691540	-4.664882
H	-4.123427	-1.290957	3.799190
H	-4.935425	-2.254996	2.541786
H	-3.983770	-0.811875	2.090344
H	-1.601748	-1.452013	4.114267
H	-1.403842	-0.849394	2.449654
H	-0.616060	-2.355378	2.934558

atom	X	Y	Z
H	-2.036836	-4.293150	3.770017
H	-3.796041	-4.308201	3.484176
H	-3.088319	-3.197454	4.668544
H	-2.484203	-6.211704	-0.223386
H	6.617859	0.968281	-0.229173
H	-4.142141	5.236226	-0.370855

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