Supplementary Information for

The Th=C double bond: an experimental and computational study of thorium poly-carbene complexes

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Experimental

General methods

All reactions and manipulations were carried out under an atmosphere of dry dinitrogen with rigid exclusion of air and moisture using standard Schlenk or cannula techniques, or in a glove box. All organic solvents were freshly distilled from sodium benzophenone ketyl immediately prior to use. Ph_2CO was purified by sublimation. $ThCl_4(DME)_2$,[1] and $[(Ph_2P{=}S)_2C]Li_2{\cdot}1.5Et_2O$ (**1**)[2] were prepared according to literature methods. All other chemicals were purchased from Aldrich Chemical Co. and Beijing Chemical Co. used as received unless otherwise noted. Infrared spectra were obtained from KBr pellets on an Avatar 360 Fourier transform spectrometer. ^1H, ^{13}C and ^{31}P NMR spectra were recorded on a Bruker AV 400 spectrometer at 400, 100 and 162 MHz, respectively. All chemical shifts were reported in δ units with reference to the residual protons of the deuterated solvents, which were internal standards, for proton and carbon chemical shifts, and to external 85% H_3PO_4 (0.00 ppm) for phosphorus chemical shifts. Melting points were measured on an X-6 melting point apparatus and were uncorrected. Elemental analyses were performed on a Vario EL elemental analyzer.

Syntheses

Preparation of $[(Ph_2P{=}S)_2C]_2Th(DME)$ (2). To a suspension of $ThCl_4(DME)_2$ (0.50 g, 0.90 mmol) in diethyl ether (20 mL) was added a diethyl ether solution (20 mL) of $[(Ph_2P{=}S)_2C]Li_2{\cdot}1.5Et_2O$ (**1**; 1.03 g, 1.80 mmol) at -78 °C with stirring. The reaction mixture was

warmed to room temperature and stirred for one day. The solvent was removed, and the resulting residue was extracted with DME (10 mL x 2). The volume of the combined filtrate was reduced to about 10 mL under vacuum, colorless crystals **2** were isolated when this solution was kept at room temperature for two days. Yield: 0.85 g (78%) (Found: C, 53.34; H, 4.17. $C_{54}H_{50}O_2P_4S_4Th$ requires C, 53.37; H, 4.15%). M.p.: 195-197 ^oC (dec.). ^1H NMR (C_6D_6): δ 7.75 (m, 16H, aryl), 7.01 (m, 8H, aryl), 6.94 (m, 16H, aryl), 3.32 (s, 4H, DME), 3.15 (s, 6H, DME). ^{13}C NMR (C_6D_6): δ 142.1 (d, J_{CP} = 77 Hz), 131.2, 129.1, 127.8 (phenyl), 72.0, 58.6 (DME); carbons of P-*C*-P were not observed. ^{31}P NMR (C_6D_6): δ 12.9 (s). IR (KBr, cm^{-1}): ν 2962 (s), 2850 (m), 1584 (w), 1413 (m), 1260 (s), 1091 (s), 1020 (s), 799 (s).

Alternate Method. To a suspension of $ThCl_4(DME)_2$ (0.50 g, 0.90 mmol) in diethyl ether (20 mL) was added a diethyl ether solution (20 mL) of $[(Ph_2P{=}S)_2C]Li_2$ (**1**) (0.42 g, 0.90 mmol) at -78 °C with stirring. The reaction mixture was warmed to room temperature and stirred for one day. Following workup procedures similar to those used above afforded colorless crystals (0.35 g, 64% yield based on **1**) identified as **2** by both spectroscopic and X-ray analyses.

Preparation of $\{[(Ph_2P{=}S)_2C]_3Th\}Li_2(DME)\cdot 2DME$ (3·2DME). To a diethyl ether solution (10 mL) of $[(Ph_2P{=}S)_2C]_2Th(DME)$ (**2**; 0.30 g, 0.25 mmol) was added a diethyl ether solution (20 mL) of $(Ph_2P{=}S)_2CLi_2\cdot 1.5Et_2O$ (**1**; 0.14 g, 0.25 mmol) at room temperature with stirring. After the solution was stirred at room temperature for one day, the solvent was removed, and the resulting residue was dissolved with DME (15 mL). The solution was filtered and reduced to about 8 mL under vacuum, colorless crystals **3**·2DME were isolated when this solution was kept at room temperature for one week. Yield: 0.35 g (75%) (Found: C 59.33; H 5.12. $C_{87}H_{90}Li_2P_6S_6Th$ requires C, 59.38; H, 5.15%). M.p.: 218-220 ^oC (dec.). ^1H NMR (C_6D_6): δ 7.28 (m, 24H, aryl), 6.92 (m, 36H, aryl), 3.20 (s, 12H, DME), 3.03 (s, 18H, DME). ^{13}C NMR (C_6D_6): δ 141.9 (d, J_{CP} = 88 Hz), 131.8, 129.1, 127.8 (phenyl), 72.0, 58.4 (DME); carbons of P-*C*-P were not observed. ^{31}P NMR (C_6D_6): δ 12.8 (s). IR (KBr, cm^{-1}): ν 3059 (w), 2940 (m), 1601 (w), 1466 (m), 1432 (s), 1241 (s), 1093 (s), 803 (s).

Alternate Method. To a suspension of $ThCl_4(DME)_2$ (0.25 g, 0.45 mmol) in diethyl ether (20 mL) was added a diethyl ether solution (20 mL) of $(Ph_2P{=}S)_2CLi_2\cdot 1.5Et_2O$ (**1**; 0.77 g, 1.35 mmol) at -78 °C with stirring. The reaction mixture was warmed to room temperature and stirred for one

day. The solvent was removed, and the resulting residue was extracted with DME (10 mL x 2). The volume of the combined filtrate was reduced to about 10 mL under vacuum, colorless crystals (0.56 g, 67% yield) were isolated when this solution was kept at room temperature for two days, which were identified as **3**·2DME by both spectroscopic and X-ray analyses.

Reaction of $[(Ph_2P=S)_2C]_2Th(DME)$ (2) with Benzophenone. A J. Young NMR tube was charged with $[(Ph_2P=S)_2C]_2Th(DME)$ (**2**; 12 mg, 0.01 mmol) and benzophenone (3.6 mg, 0.02 mmol) in C_6D_6 (0.5 mL). This sample was maintained at 70 °C, after 2 h, white precipitate (ThO_2) appeared, and the resonances due to $Ph_2C=C[P(S)Ph_2]_2$ (^{1}H NMR (C_6D_6): δ 8.21 (br s, 4 H, aryl), 7.10-6.72 (m, 16 H); ^{31}P NMR (C_6D_6): δ 40.7 (s))[3] were observed by ^{1}H and ^{31}P NMR spectroscopy (100% conversion).

Reaction of $\{[(Ph_2P=S)_2C]_3Th\}Li_2(DME)$ (3) with Benzophenone. A J. Young NMR tube was charged with $\{[(Ph_2P=S)_2C]_3Th\}Li_2(DME)$·2DME (**3**; 19 mg, 0.01 mmol) and benzophenone (5.4 mg, 0.03 mmol) in C_6D_6 (0.5 mL). This sample was maintained at 70 °C overnight, white precipitate (ThO_2) appeared, and the resonances due to $Ph_2C=C[P(S)Ph_2]_2$[3] were observed by ^{1}H and ^{31}P NMR spectroscopy (100% conversion).

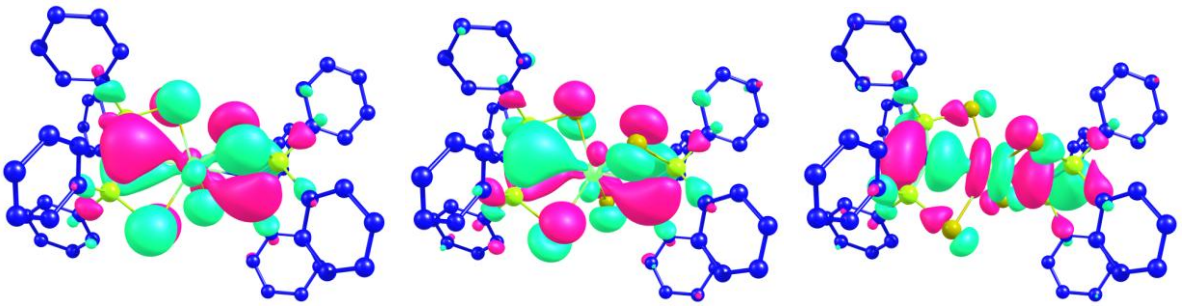
X-Ray crystallography

Single-crystal X-ray diffraction measurements were carried out on a Bruker Smart APEX II CCD diffractometer at 110(2) or 150(2) K using graphite monochromated Mo Kα radiation (λ = 0.71070 Å). An empirical absorption correction was applied using the SADABS program.[5] All structures were solved by direct methods and refined by full-matrix least squares on F^2 using the SHELXL-97 program package.[6] All the hydrogen atoms were geometrically fixed using the riding model. The crystal data and experimental data for **2** and **3** are summarized in Table 1. Selected bond lengths and angles are listed in Table 2.

Computational Methods.

All calculations were carried out with the Gaussian 09 program (G09),[7] employing the Becke-3-Lee-Yang-Parr (B3LYP) method with standard 6-31G(d) basis set for C, H, O, P and S elements

and Stuttgart RLC ECP from EMSL basis set exahange (https://bse.pnl.gov/bse/portal) for Th element,[8] to fully optimize the geometries of the complexes.



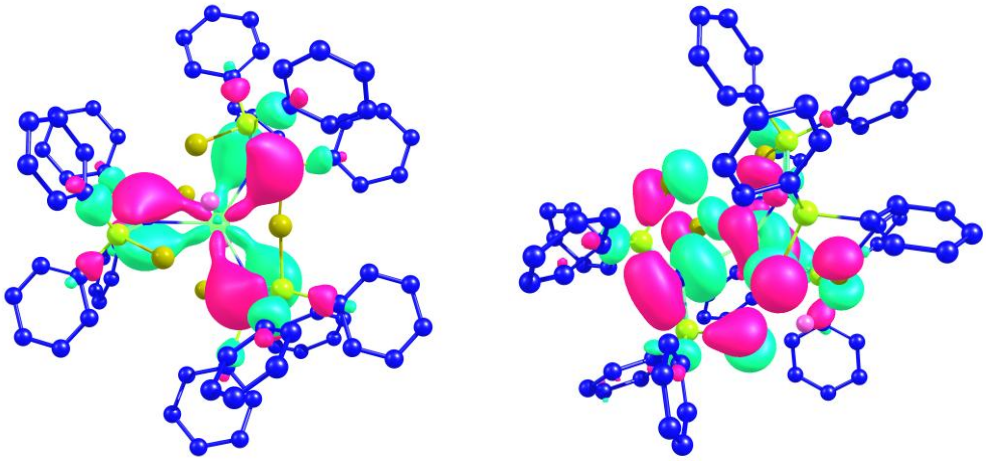
HOMO (π-orbital)	HOMO-1 (π-orbital)	HOMO-2 (σ-orbital)
(238, e = - 0.1961 au)	(237, e = - 0.1974 au)	(236, e = -0.1980 au)

Fig. 1. Isosurfaces (contour drawn at the 0.025 level for all of them) and energies of the MOs of **2a** (obtained from DFT calculation, the hydrogen atoms omitted for clarity).

In the proposed base-free bis-carbene complex $(Ph_2P{=}S)_2C{=}Th{=}C(Ph_2P{=}S)_2$ (**2a**), the calculated values for the Th-C distance is 2.454 Å and for the angles C-Th-C is 180.0°, and the Mayer bond order is 1.03. The Mulliken analysis reveals that the thorium atom bears a charge of +0.19, and each carbon atom has a charge of -0.47. Each thorium-carbon interaction is described by the two highest molecular orbitals (MOs), which are both mainly centred on the carbon atom. The HOMO-2 describes the σ interaction between C and Th atoms, whereas the HOMO describes the π interaction (Figure 1). A natural bond orbital (NBO) analysis reveals that the donation from a carbon 2p orbital (0.69 P_y + 0.72 P_z; 88.3%) to a thorium hybrid orbital (11.7%) having 61.4% 6d and 32.1% 5f character forms the Th=C σ bond. On the other hand, the donor-acceptor interaction (Th= C π bond) between the carbon lone pair (sp hybrid orbital with 0.35 S - 0.94 P_x) and the thorium fragment is small since the thorium hybrid orbital is less than 5%.

The calculated value for the Th-C distance is 2.555 Å and for the angle C-Th-C is 120.2° which compare very favourably with experimental values for **3** of 2.527(4), 2.552(4) and 2.549(4) Å and 117.6(1), 121.1(1) and 121.2(1)°. Each thorium-carbon interaction is described by the two highest molecular orbitals, which are both mainly centred on the carbon atom, and the Mayer bond order is 0.87. The Mulliken analysis reveals that the thorium atom bears a charge of +0.45, and each carbon atom has a charge of -0.46. The HOMO-3 describes the σ interaction between C and Th atoms,

whereas the HOMO-2 describes the π interaction (Figure 2). A natural bond orbital (NBO) analysis reveals that the donation from a carbon 2p orbital (-0.23 P_x + 0.86 P_y + 0.46 P_z; 90.4%) to a thorium hybrid orbital (9.6%) having 44.1% 6d and 48.6% 5f character forms the Th=C σ bond. On the other hand, the donor-acceptor interaction (Th= C π bond) between the carbon lone pair (sp hybrid orbital with 0.40 S + 0.88 P_x + 0.24 P_y) and the thorium fragment is small since the thorium hybrid orbital is less than 5%.



HOMO-2 (π-orbital) (355, e = -0.1815 au)

HOMO-3 (σ-orbital) (354, e = -0.1982 au)

Fig. 2. Isosurfaces (contour drawn at the 0.025 level for left and 0.030 for right) and energies of the MOs of **3** (obtained from DFT calculation, the hydrogen atoms omitted for clarity).

References

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Table 1 Crystal data and experimental parameters for compounds **2** and **3**

compound	**2**	**3**·2DME
formula	$C_{54}H_{50}O_2P_4S_4Th$	$C_{87}H_{90}Li_2O_6P_6S_6Th$
formula weight	1215.10	1855.69
crystal system	triclinic	orthorhombic
space group	*P*(-1)	*Pbca*
a (Å)	10.883(1)	21.048(1)
b (Å)	14.676(2)	23.538(1)
c (Å)	17.335(2)	35.031(2)
α (deg)	70.00(1)	90
β (deg)	88.65(1)	90
γ (deg)	75.20(1)	90
V (Å^3)	2509.3(5)	17354.9(15)
Z	2	8
$D_{calc.}$ (g/cm^3)	1.608	1.420
size (mm)	0.25 x 0.12 x 0.08	0.27 x 0.25 x 0.20
F(000)	1208	7536
2θ range (deg)	4.26 to 50.50	3.48 to 55.22
no. of reflections collected	12837	100950
no. of unique reflections [$R_{(int)}$]	8998 (0.0520)	20035 (0.1101)
no. of observed reflections	7149	12897
absorbed corrections (T_{max}, T_{min})	0.78, 0.49	0.69, 0.61
R	0.053	0.044
R_w	0.098	0.086
*wR*2 (all data)	0.108	0.100
gof	0.97	1.01

Table 2 Selected bond distances (Å) and bond angles (deg) for compounds **2** and **3**

Compound **2**			
C(13)-P(1)	1.668(7)	C(13)-P(2)	1.669(7)
C(38)-P(3)	1.682(8)	C(38)-P(4)	1.675(7)
P(1)-S(1)	2.041(3)	P(2)-S(2)	2.028(3)
P(3)-S(3)	2.021(3)	P(4)-S(4)	2.024(3)
C(13)-Th(1)	2.498(7)	C(38)-Th(1)	2.485(7)
O(1)-Th(1)	2.547(5)	O(2)-Th(1)	2.601(5)
P(1)-Th(1)	3.330(2)	P(2)-Th(1)	3.344(2)
P(3)-Th(1)	3.371(2)	P(4)-Th(1)	3.316(2)
S(1)-Th(1)	2.875(2)	S(2)-Th(1)	2.931(2)
S(3)-Th(1)	3.007(2)	S(4)-Th(1)	2.909(2)
P(1)-C(13)-P(2)	149.3(5)	P(3)-C(38)-P(4)	141.9(4)
S(1)-Th(1)-S(2)	132.1(1)	S(3)-Th(1)-S(4)	129.0(1)
sum angle of C(13)	358.6(5)	sum angle of C(38)	352.3(4)
C(13)-Th(1)-C(38)	142.7(2)		
Compound **3**			
C(1)-P(1)	1.660(5)	C(1)-P(2)	1.663(5)
C(26)-P(3)	1.655(4)	C(26)-P(4)	1.675(4)
C(51)-P(5)	1.666(5)	C(51)-P(6)	1.657(5)
P(1)-S(1)	2.038(2)	P(2)-S(2)	2.036(2)
P(3)-S(3)	2.039(2)	P(4)-S(4)	2.031(2)
P(5)-S(5)	2.027(2)	P(6)-S(6)	2.035(2)
S(1)-Li(1)	2.433(1)	S(3)-Li(1)	2.482(9)
S(5)-Li(1)	2.419(9)	S(2)-Li(2A)	2.423(9)
S(4)-Li(2A)	2.460(8)	S(6)-Li(2A)	2.430(9)
O(5)-Li(1)	1.919(9)	O(6)-Li(2)	1.896(9)
C(1)-Th(1)	2.552(4)	C(26)-Th(1)	2.527(4)
C(51)-Th(1)	2.549(4)	P(1)-Th(1)	3.427(1)
P(2)-Th(1)	3.456(1)	P(3)-Th(1)	3.436(1)
P(4)-Th(1)	3.433(1)	P(5)-Th(1)	3.447(1)
P(6)-Th(1)	3.440(1)	S(1)-Th(1)	3.026(1)
S(2)-Th(1)	3.074(1)	S(3)-Th(1)	3.090(1)
S(4)-Th(1)	3.060(1)	S(5)-Th(1)	3.094(1)
S(6)-Th(1)	3.085(1)	Th(1)-Li(1)	3.431(8)
Th(1)-Li(2A)	3.424(8)	P(1)-C(1)-P(2)	144.9(3)
P(3)-C(26)-P(4)	143.2(3)	P(5)-C(51)-P(6)	144.2(3)
S(1)-Th(1)-S(2)	126.7(1)	S(3)-Th(1)-S(4)	126.3(1)
S(5)-Th(1)-S(6)	125.5(1)	sum angle of C(1)	359.9(3)
sum angle of C(26)	359.7(3)	sum angle of C(51)	359.9(3)
C(1)-Th(1)-C(26)	121.2(1)	C(1)-Th(1)-C(51)	121.1(1)
C(26)-Th(1)-C(51)	117.6(1)	Li(1)-Th(1)-Li(2A)	178.0(2)

Table 3. The optimized Cartesian Coordinates(in Å) of stationary points for the studied complexes.

complex	Cartesian coordinates					
2	C	-2.61419	2.89295	-0.36945	H	4.85240 -0.32382 -3.84094
	C	-2.34381	3.07692	0.99260	C	4.70183 1.70393 -4.53777
	H	-2.07730	2.22424	1.60685	H	5.35927 1.53525 -5.38671
	C	-2.41352	4.35215	1.55941	C	4.14429 2.96819 -4.32173
	H	-2.20976	4.47959	2.61910	H	4.36954 3.78498 -5.00262
	C	-2.74845	5.45338	0.76953	C	3.29683 3.17707 -3.23314
	H	-2.80426	6.44506	1.21103	H	2.85776 4.15557 -3.05963
	C	-3.01385	5.27756	-0.59189	C	3.00675 2.12721 -2.35789
	H	-3.27355	6.13145	-1.21215	H	2.34056 2.28825 -1.51819
	C	-2.94726	4.00510	-1.15949	C	2.35776 -0.11727 0.01021
	H	-3.15350	3.87953	-2.21856	C	3.82100 0.17520 2.61523
	C	-3.79286	1.17295	-2.36491	C	4.49583 -1.02607 2.36863
	C	-3.56970	0.73738	-3.67796	H	4.29768 -1.57063 1.45156
	H	-2.55725	0.50718	-3.99696	C	5.42546 -1.51650 3.29076
	C	-4.63610	0.61833	-4.57365	H	5.94971 -2.44567 3.08351
	H	-4.44933	0.28617	-5.59154	C	5.68260 -0.81189 4.46713
	C	-5.93334	0.93539	-4.16682	H	6.40440 -1.19269 5.18492
	H	-6.76150	0.84628	-4.86486	C	5.00918 0.38775 4.72139
	C	-6.16362	1.37582	-2.85991	H	5.20486 0.93914 5.63722
	H	-7.17036	1.63084	-2.53972	C	4.08420 0.87947 3.80159
	C	-5.10093	1.49389	-1.96421	H	3.56417 1.81098 4.00778
	H	-5.28926	1.84648	-0.95352	C	2.99662 2.56650 1.22847
	C	-2.34308	-0.08593	-0.04767	C	4.34098 2.93509 1.05773
	C	-4.60646	-1.93763	0.57757	H	5.12526 2.18642 1.13132
	C	-4.90311	-2.02488	-0.78691	C	4.68251 4.26425 0.80505
	H	-4.32815	-1.43785	-1.49502	H	5.72660 4.53808 0.67848
	C	-5.93608	-2.85484	-1.23415	C	3.68547 5.23955 0.71924
	H	-6.16210	-2.90883	-2.29593	H	3.95219 6.27493 0.52435
	C	-6.67630	-3.60454	-0.31960	C	2.34643 4.88027 0.88874
	H	-7.47915	-4.25009	-0.66608	H	1.56559 5.63350 0.82704
	C	-6.38448	-3.52231	1.04644	C	2.00203 3.55100 1.14345
	H	-6.95848	-4.10481	1.76228	H	0.96071 3.27636 1.28173
	C	-5.35627	-2.69379	1.49316	C	1.43009 -3.47409 2.11311
	H	-5.13199	-2.63775	2.55500	H	0.62916 -3.61672 2.84671
	C	-4.05894	0.20918	2.41703	H	1.96939 -2.55247 2.33057
	C	-5.31277	0.77265	2.13030	H	2.12084 -4.32526 2.13794
	H	-5.83255	0.50792	1.21346	C	0.11831 -4.48993 0.39648
	C	-5.90803	1.66261	3.02550	H	-0.77634 -4.55746 1.02587
	H	-6.88052	2.08979	2.79525	H	0.72851 -5.39391 0.52490
	C	-5.25907	1.99703	4.21698	C	-0.25693 -4.35081 -1.06198
	H	-5.72497	2.68751	4.91505	H	0.63442 -4.33504 -1.70007
	C	-4.01425	1.43600	4.51081	H	-0.90061 -5.19255 -1.34880
	H	-3.50842	1.68577	5.43974	C	-1.55733 -2.99321 -2.54107
	C	-3.41642	0.54564	3.61629	H	-0.77904 -3.00799 -3.31193
	H	-2.45351	0.09983	3.84725	H	-2.07969 -2.03675 -2.55699
	C	4.73691	-1.42732	-1.25825	H	-2.27162 -3.80816 -2.70643
	C	4.80152	-2.82584	-1.31483	O	0.88231 -3.34130 0.79061
	H	3.90540	-3.38814	-1.56034	O	-0.97772 -3.12316 -1.23496
	C	6.00812	-3.48876	-1.07555	P	-2.42209 1.22069 -1.12409
	H	6.04684	-4.57375	-1.12917	P	-3.22123 -0.87112 1.17227

	C 7.16245 -2.76084 -0.77937 H 8.10164 -3.27657 -0.59755 C 7.10782 -1.36521 -0.72516 H 8.00382 -0.79236 -0.50137 C 5.90340 -0.70231 -0.96233 H 5.87509 0.38344 -0.92633 C 3.56869 0.86142 -2.56344 C 4.41570 0.65512 -3.66472	P 3.12603 -0.53419 -1.44244 P 2.54618 0.78663 1.42871 S -0.60479 1.14681 -2.09991 S -1.85384 -2.07281 2.12971 S 1.77917 -1.74974 -2.42264 S 0.70653 0.63748 2.36115 Th -0.00033 -0.92228 -0.05474
2a	C 2.51887 0.08171 0.02970 C 4.19182 1.18998 -2.11678 C 3.71258 0.94634 -3.39211 H 2.78162 1.02649 -3.56534 C 4.58442 0.58339 -4.43736 H 4.24524 0.44223 -5.31408 C 5.92709 0.43238 -4.18450 H 6.52181 0.16942 -4.87883 C 6.39407 0.66987 -2.92113 H 7.32233 0.57050 -2.74400 C 5.54976 1.04807 -1.89045 H 5.90434 1.20994 -1.02588 C 3.90941 2.67055 0.29458 C 4.34768 3.88154 -0.26329 H 4.21759 4.04292 -1.19141 C 4.96730 4.84205 0.51129 H 5.25668 5.65736 0.12150 C 5.15791 4.60367 1.87010 H 5.57520 5.26337 2.41278 C 4.74380 3.40082 2.43599 H 4.88267 3.23522 3.35989 C 4.11871 2.43975 1.63472 H 3.83435 1.61737 2.02063 C 4.00907 -2.47243 -0.32825 C 4.11371 -2.23553 -1.69342 H 3.69510 -1.47168 -2.07520 C 4.82489 -3.11064 -2.50016 H 4.90192 -2.93499 -3.42953 C 5.40626 -4.19652 -1.98317 H 5.88484 -4.79034 -2.54880 C 5.31664 -4.46276 -0.63538 H 5.73109 -5.23770 -0.27205 C 4.61519 -3.59172 0.19389 H 4.55532 -3.76992 1.12384 C 4.16271 -1.19700 2.18192 C 5.47712 -0.84939 1.99762 H 5.80302 -0.71137 1.11573 C 6.33910 -0.69901 3.08055 H 7.23927 -0.43008 2.93669 C 5.88653 -0.93754 4.35524 H 6.48103 -0.86208 5.09563 C 4.59442 -1.28185 4.55147 H 4.28258 -1.44245 5.43628 C 3.70343 -1.40885 3.46959	H -4.67269 0.45331 5.33527 C -6.17753 0.31414 4.06450 H -6.82549 0.09442 4.72259 C -6.54906 0.40687 2.73000 H -7.44540 0.23964 2.46836 C -5.59366 0.74685 1.78632 H -5.84560 0.81916 0.87454 C -3.91374 2.63377 -0.11643 C -4.21943 3.83732 0.48824 H -3.98529 3.97491 1.39729 C -4.86415 4.85722 -0.21322 H -5.04715 5.68607 0.21580 C -5.23111 4.66048 -1.51614 H -5.67771 5.34550 -1.99974 C -4.94539 3.45849 -2.11800 H -5.20612 3.31949 -3.02233 C -4.28799 2.44548 -1.44281 H -4.09351 1.62677 -1.88142 C -3.77816 -2.68253 0.14511 C -4.03686 -2.48417 1.47927 H -3.80984 -1.65662 1.88326 C -4.63034 -3.48630 2.24478 H -4.80020 -3.33673 3.16885 C -4.97148 -4.69427 1.66379 H -5.38870 -5.37517 2.17868 C -4.69930 -4.90070 0.32738 H -4.91812 -5.73512 -0.07092 C -4.10692 -3.90193 -0.44564 H -3.92778 -4.05078 -1.36751 C -4.21163 -1.10334 -2.19548 C -5.59303 -1.21081 -1.93388 H -5.90195 -1.49169 -1.08172 C -6.49515 -0.90183 -2.94153 H -7.42518 -0.97426 -2.76324 C -6.08963 -0.50478 -4.15632 H -6.73385 -0.31851 -4.82980 C -4.74193 -0.36619 -4.43715 H -4.45954 -0.05654 -5.29032 C -3.79871 -0.68388 -3.45756 H -2.87154 -0.61544 -3.65419 P 3.04004 1.45406 -0.73128 P 3.05234 -1.34384 0.73022 P -3.06255 1.32403 0.82949 P -2.99613 -1.35308 -0.85171

	H 2.79414 -1.63998 3.62182 C -2.52307 -0.00414 -0.01555 C -4.28213 0.98403 2.14563 C -3.92035 0.88207 3.48423 H -3.02619 1.04430 3.76286 C -4.91213 0.53400 4.41976	S 1.37957 2.35819 -1.49291 S 1.38984 -2.31501 1.37728 S -1.44273 2.14527 1.73019 S -1.32872 -2.10965 -1.74158 Th -0.00354 0.03876 0.00706
3	C -2.46831 -0.65736 0.00360 C -4.76352 0.89344 -1.17787 C -4.70803 2.28907 -1.05633 H -3.75914 2.79881 -1.19119 C -5.86507 3.02006 -0.77857 H -5.81054 4.10299 -0.69824 C -7.08901 2.36704 -0.61679 H -7.98910 2.93764 -0.40346 C -7.15299 0.97723 -0.73909 H -8.10328 0.46260 -0.62274 C -5.99850 0.24484 -1.01959 H -6.06188 -0.83475 -1.12554 C -3.78317 -1.37408 -2.63235 C -4.38661 -0.95804 -3.83139 H -4.53029 0.10131 -4.02676 C -4.79726 -1.89769 -4.77473 H -5.26169 -1.56710 -5.70021 C -4.61218 -3.26304 -4.53009 H -4.93396 -3.99528 -5.26623 C -4.01253 -3.68055 -3.34277 H -3.86441 -4.73902 -3.14666 C -3.59429 -2.73920 -2.39730 H -3.11421 -3.06288 -1.48174 C -3.95270 -0.69764 2.64429 C -4.46068 0.58472 2.41652 H -4.19942 1.10849 1.50493 C -5.28930 1.19210 3.36488 H -5.68107 2.18768 3.17485 C -5.60671 0.52593 4.54778 H -6.24815 1.00014 5.28623 C -5.09493 -0.75464 4.78536 H -5.33698 -1.27670 5.70751 C -4.27358 -1.36416 3.83913 H -3.87730 -2.35811 4.02893 C -3.67943 -3.14934 1.18475 C -5.07297 -3.19998 1.02127 H -5.66504 -2.29450 1.12351 C -5.70996 -4.40939 0.73988 H -6.78987 -4.43503 0.61940 C -4.96347 -5.58395 0.62180 H -5.46038 -6.52661 0.40791 C -3.57745 -5.54257 0.78849 H -2.99171 -6.45526 0.71063 C -2.93738 -4.33303 1.06722 H -1.86102 -4.30319 1.20501 C 1.81009 -1.80433 -0.00347	C 3.18173 -4.05313 4.77362 H 3.74942 -4.00643 5.69938 C 3.30582 -3.03311 3.83247 H 3.96823 -2.19441 4.02955 C 4.56897 -1.61284 1.19105 C 5.30976 -2.79367 1.02304 H 4.81982 -3.75934 1.11477 C 6.67755 -2.73962 0.75129 H 7.23989 -3.66154 0.62777 C 7.32324 -1.50545 0.64715 H 8.38949 -1.46370 0.44062 C 6.59410 -0.32662 0.81781 H 7.09285 0.63719 0.75101 C 5.22461 -0.37814 1.08694 H 4.66062 0.53844 1.22908 C 0.66309 2.46696 0.00165 C 3.14198 3.67890 -1.20028 C 4.32630 2.93716 -1.08811 H 4.29650 1.86064 -1.22481 C 5.53738 3.57758 -0.81668 H 6.45042 2.99181 -0.74361 C 5.57963 4.96370 -0.65176 H 6.52330 5.46095 -0.44315 C 4.40439 5.71003 -0.76463 H 4.43073 6.79010 -0.64557 C 3.19346 5.07281 -1.03883 H 2.28750 5.66486 -1.13644 C 0.67873 3.95131 -2.64043 C 1.33139 4.26055 -3.84582 H 2.31906 3.85432 -4.04720 C 0.71600 5.08244 -4.78781 H 1.22737 5.31525 -5.71829 C -0.55676 5.60626 -4.53533 H -1.03562 6.24817 -5.27036 C -1.20936 5.30022 -3.34187 H -2.19893 5.70139 -3.14034 C -0.59633 4.47082 -2.39787 H -1.11023 4.21859 -1.47819 C 1.38767 3.75859 2.64447 C 2.75276 3.58699 2.39602 H 3.07420 3.12444 1.47054 C 3.69699 3.99886 3.34135 H 4.75541 3.86429 3.13531 C 3.28259 4.57402 4.54189 H 4.01735 4.89025 5.27793 C 1.91744 4.74131 4.79991

	C 1.62635 -4.56569 -1.19596 C 0.39680 -5.22956 -1.08387 H -0.52473 -4.67186 -1.21877 C 0.35613 -6.59951 -0.81518 H -0.60387 -7.10472 -0.74217 C 1.54081 -7.32083 -0.65259 H 1.50753 -8.38744 -0.44635 C 2.76997 -6.66696 -0.76485 H 3.69630 -7.22327 -0.64730 C 2.81325 -5.29887 -1.03675 H 3.77519 -4.80309 -1.13541 C 3.07464 -2.56214 -2.64627 C 3.01499 -3.27825 -3.85372 H 2.17084 -3.93258 -4.05462 C 4.03191 -3.14994 -4.79775 H 3.97730 -3.70596 -5.73014 C 5.12034 -2.30764 -4.54469 H 5.91359 -2.20914 -5.28135 C 5.18329 -1.59431 -3.34841 H 6.02484 -0.93723 -3.14639 C 4.16100 -1.71667 -2.40251 H 4.19983 -1.15028 -1.47979 C 2.57494 -3.08241 2.63335 C 1.71851 -4.16144 2.39559 H 1.14066 -4.19255 1.47977 C 1.60006 -5.18676 3.33871 H 0.93433 -6.02256 3.14117 C 2.32850 -5.13434 4.52633 H 2.23322 -5.93011 5.26071	H 1.58929 5.18650 5.73563 C 0.97480 4.33744 3.85655 H -0.08452 4.46753 4.06170 C -0.87394 4.76160 1.19665 C -0.21834 5.99483 1.05451 H 0.86069 6.05200 1.16883 C -0.94329 7.15511 0.77876 H -0.42346 8.10397 0.67457 C -2.33244 7.09878 0.64558 H -2.89719 8.00349 0.43618 C -2.99233 5.87646 0.79080 H -4.07482 5.82760 0.70165 C -2.26877 4.71346 1.06315 H -2.78383 3.76532 1.18297 P -3.22285 -0.11125 -1.40663 P -2.84291 -1.51135 1.41319 P 1.70824 -2.72707 -1.41530 P 2.73093 -1.70836 1.40970 P 1.50249 2.84186 -1.41561 P 0.12095 3.21359 1.41645 S -1.84038 1.12326 -2.33833 S -1.02376 -1.89564 2.33369 S -0.06401 -2.15739 -2.33097 S 2.15184 0.05495 2.33741 S 1.88016 1.02381 -2.34172 S -1.12201 1.83235 2.33961 Th 0.00012 -0.00079 -0.00026 Li -0.00931 -0.00836 -3.36025 Li 0.00136 -0.00387 3.35964