

Supporting information

for

Synthesis of *P,P*-bidentate caged phosphines via tungsten pentacarbonyl-promoted cycloaddition reactions of 1-alkyl-1,2-diphospholes

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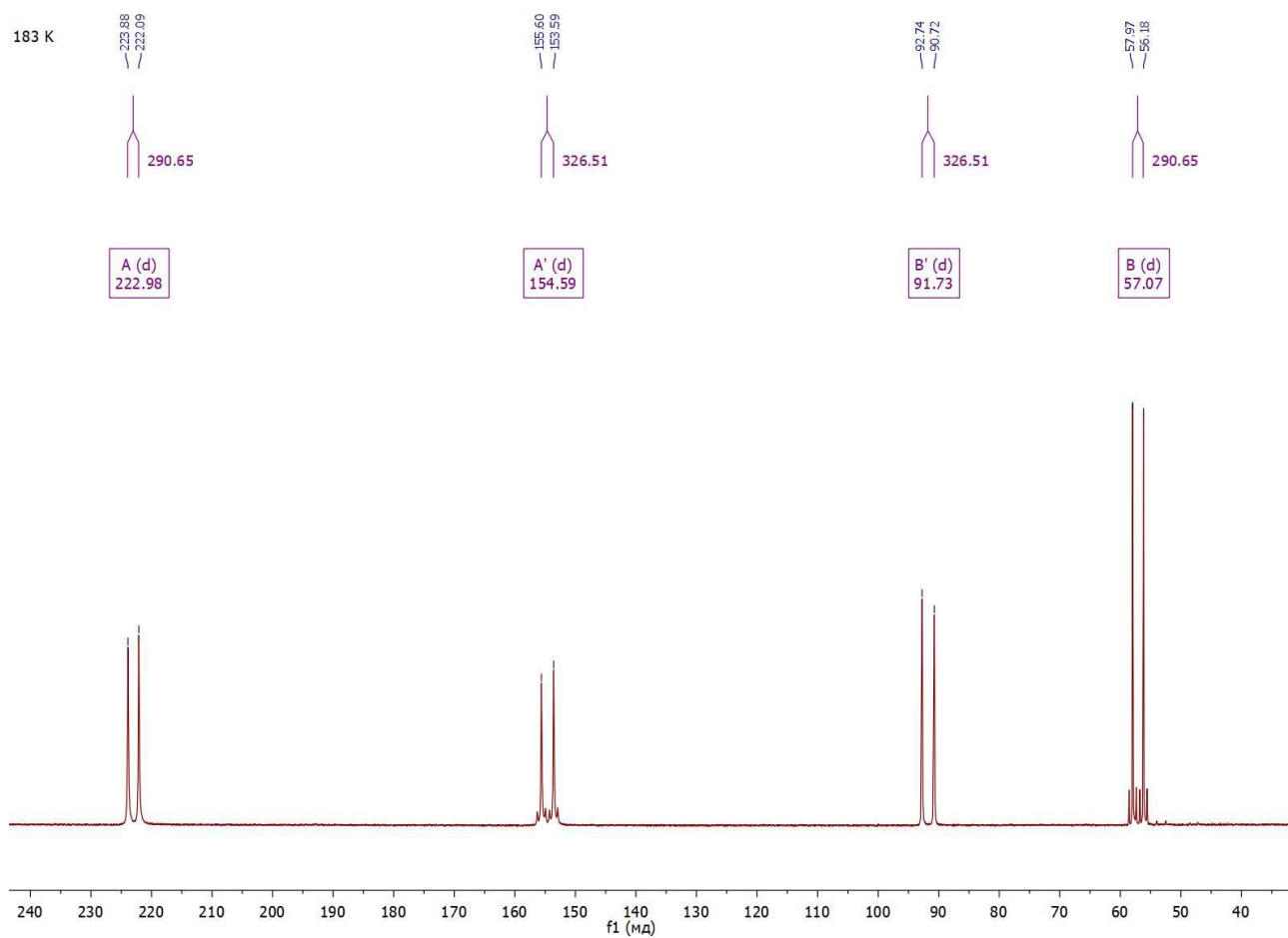


Figure S1. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2b** (162.0 MHz, -90 °C, THF- d_8)

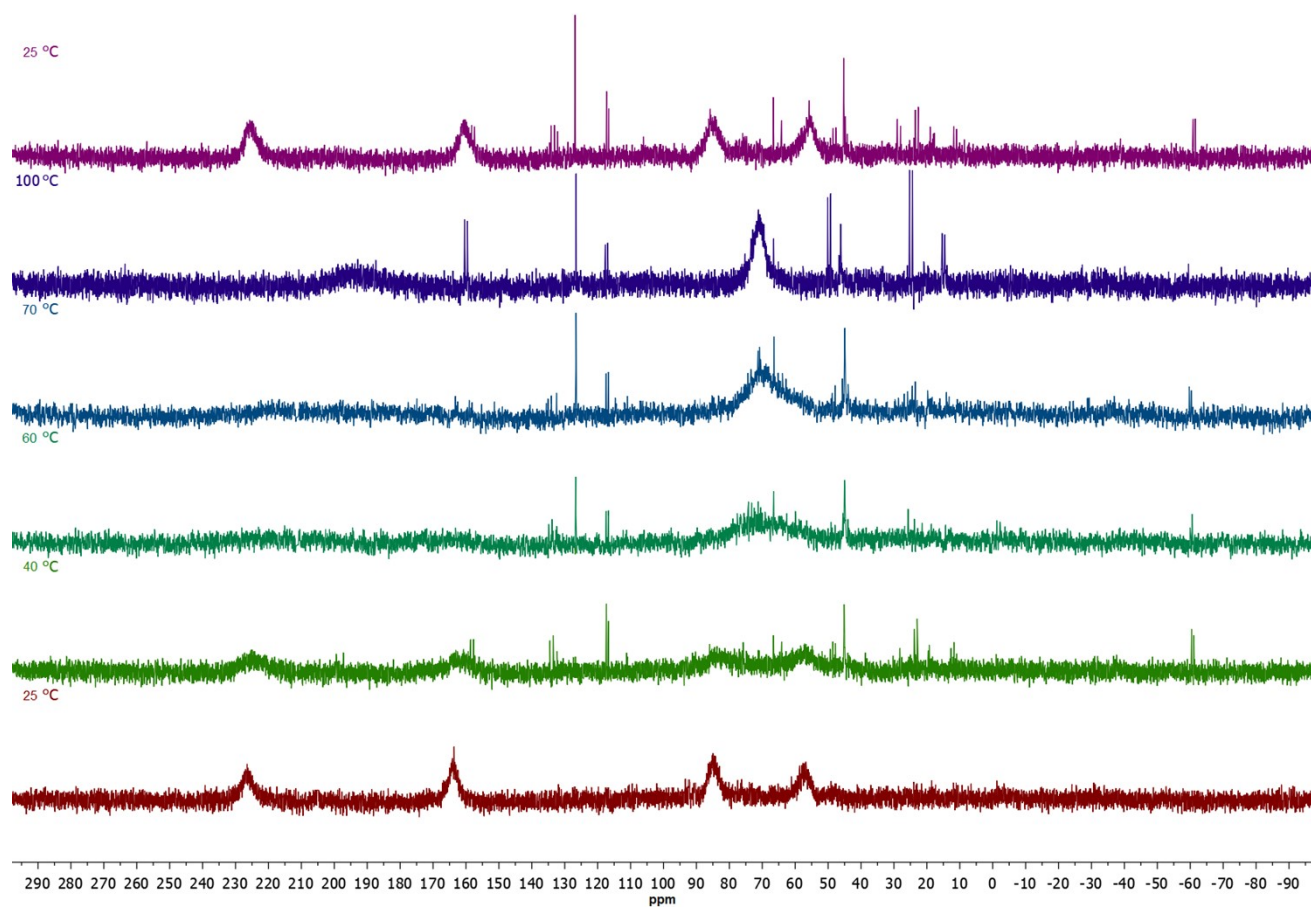


Figure S2. Variable-temperature $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of 2b/2b' (242.9 MHz, 25 to 100 °C, Toluene- d_8)

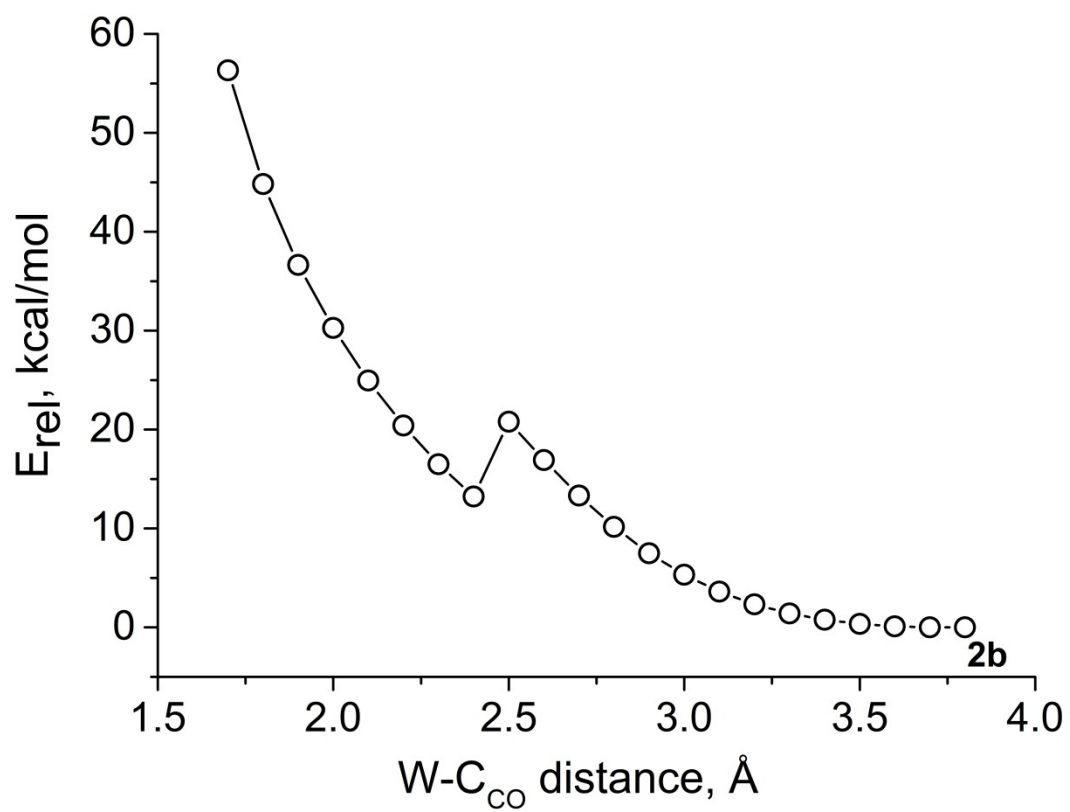


Figure S3. Energy profile of **2b** at $W-C_{CO}$ distance

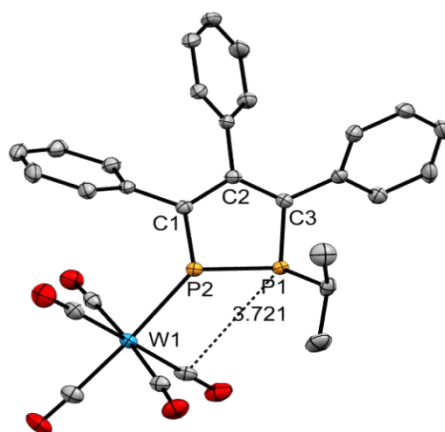


Figure S4. Molecular structure and labelling scheme of compound **2b**. Hydrogen atoms are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

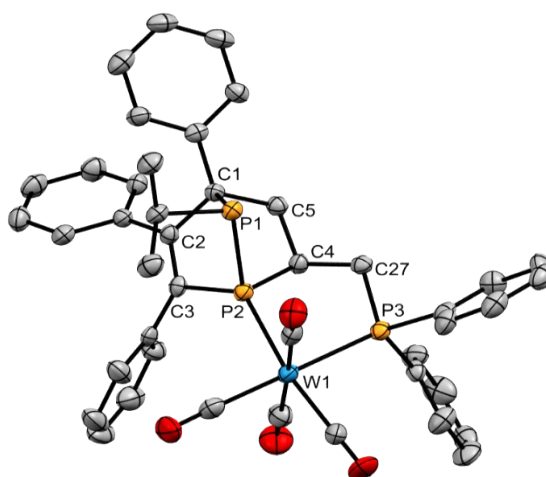


Figure S5. Molecular structure and labelling scheme of compound **3b**. Hydrogen atoms are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

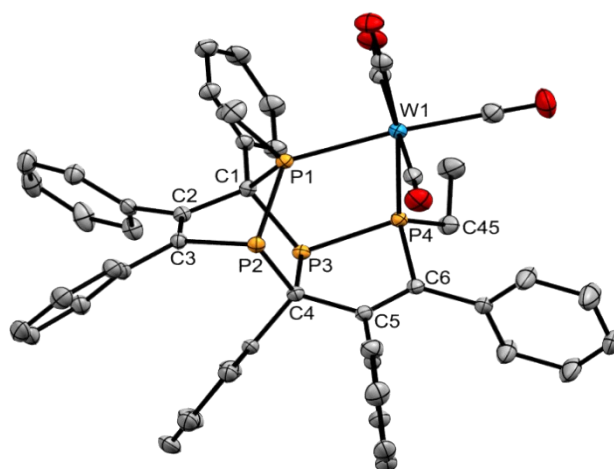


Figure S6. Molecular structure and labelling scheme of compound **4a**. Hydrogen atoms are omitted for clarity and displacement ellipsoids are drawn at the 50% probability level.

Table S1. Fundamental crystal structure parameters

Compound	2b	3b	4a
Empirical formula	C ₂₉ H ₂₂ O ₅ P ₂ W	C _{53.50} H ₄₉ O ₄ P ₃ W	C ₅₀ H ₄₀ O ₄ P ₄ W
Molecular formula	C ₂₉ H ₂₂ O ₅ P ₂ W	C ₄₃ H ₃₇ O ₄ P ₃ W · 1.5 toluene	C ₅₀ H ₄₀ O ₄ P ₄ W
Formula weight	696.25	1032.68	1012.55
Temperature [K]	130(2)	130(2)	130(2)
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> $\bar{1}$
Unit cell dimensions			
a [pm]	2184.84(3)	3676.7(1)	1119.96(1)
b [pm]	662.65(1)	930.53(2)	1257.70(2)
c [pm]	1952.50(3)	2827.16(7)	1703.15(2)
α [deg]	90	90	96.854(1)
β [deg]	106.818(1)	106.002(3)	105.569(1)
γ [deg]	90	90	108.354(1)
Volume [nm ³]	2.70589(7)	9.2976(4)	2.13821(5)
Z	4	8	2
ρ (calc.) [Mg/m ³]	1.709	1.475	1.573
μ [mm ⁻¹]	4.424	2.633	2.897
F(000)	1360	4168	1012
Crystal size [mm ³]	0.38 · 0.25 · 0.20	0.32 · 0.07 · 0.05	0.39 · 0.20 · 0.14
Θ_{\min} - Θ_{\max} [deg]	1.947 - 30.507	1.499 - 26.372	1.921 - 30.508
	-31 ≤ h ≤ 24	-45 ≤ h ≤ 44	-15 ≤ h ≤ 15
Index ranges	-9 ≤ k ≤ 8	-11 ≤ k ≤ 11	-17 ≤ k ≤ 17
	-27 ≤ l ≤ 27	-35 ≤ l ≤ 35	-24 ≤ l ≤ 24
Reflections collected	29001	39224	95272
Independent reflections [R _(int)]	8274 [0.0300]	9519 [0.0742]	13023 [0.0386]
Completeness (Θ [deg])	100.0 % (30.51)	100.0 % (26.37)	100.0 % (30.51)
T _{Min} / T _{Max}	1.00000 / 0.79968	1.00000 / 0.87423	1.00000 / 0.85427
Restraints / parameters	0 / 336	61 / 590	0 / 534
Goof [on F ²]	1.077	1.033	1.076
R1, wR2 [I > 2 σ (I)]	0.0221, 0.0448	0.0414, 0.0836	0.0208, 0.0471
R1, wR2 (all data)	0.0270, 0.0467	0.0653, 0.0921	0.0235, 0.0480
Residual electron density [e·Å ⁻³]	1.662 / -0.756	1.332 / -0.669	1.240 / -0.675
Comments	-	†	-
CCDC deposition number	2300839	2300840	2300841

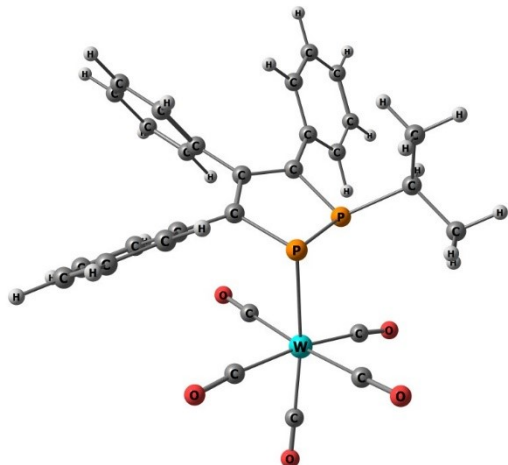
†: The toluene solvent molecule is located disordered on a twofold axis.

Table S2. Cartesian coordinates and total energies of optimized structures **2b**, **2b'**, and **2b_TS**

2b			
Charge : 0			
Multiplicity : 1			
Total energy: -18808.6908120454 a.u.			
74	-2.890058000	-0.285476000	-0.175677000
15	-0.407071000	-0.349826000	0.286397000
15	0.955405000	-1.896632000	-0.420001000
8	-2.416555000	-2.509747000	-2.437540000
8	-3.419022000	-2.620683000	1.954208000
8	-5.960125000	-0.287923000	-0.949112000
8	-3.532097000	1.871177000	2.110880000
8	-2.409024000	2.064325000	-2.313712000
6	0.814761000	0.900780000	0.176592000
6	2.189361000	0.481236000	-0.026193000
6	2.438190000	-0.884286000	-0.218418000
6	1.112518000	-3.315577000	0.827377000
1	2.012964000	-3.839702000	0.434493000
6	1.382068000	-2.869554000	2.266334000
1	0.516964000	-2.313647000	2.681633000
1	2.277966000	-2.222657000	2.339956000
1	1.551896000	-3.758802000	2.910292000
6	-0.094060000	-4.255073000	0.707755000
1	0.085052000	-5.171433000	1.307604000
1	-0.284472000	-4.565374000	-0.338991000
1	-1.019081000	-3.786349000	1.100225000
6	0.401890000	2.323844000	0.250405000
6	-0.354800000	2.800430000	1.345850000
1	-0.593578000	2.114843000	2.172822000
6	-0.782234000	4.134855000	1.398222000
1	-1.372287000	4.482420000	2.259689000
6	-0.460931000	5.018570000	0.356452000
1	-0.798033000	6.065600000	0.394927000
6	0.293519000	4.559264000	-0.736203000
1	0.545066000	5.244737000	-1.559857000
6	0.724992000	3.227938000	-0.789711000
1	1.306719000	2.873285000	-1.652999000
6	3.293549000	1.488233000	-0.036283000
6	3.471901000	2.384068000	1.041540000
1	2.783058000	2.343203000	1.898414000
6	4.520264000	3.315096000	1.030830000
1	4.647744000	4.000930000	1.882400000
6	5.401071000	3.376236000	-0.061064000

1	6.220165000	4.111503000	-0.070648000
6	5.228474000	2.496646000	-1.141880000
1	5.910921000	2.541263000	-2.004502000
6	4.186376000	1.558839000	-1.128752000
1	4.053362000	0.870678000	-1.977040000
6	3.753959000	-1.550716000	-0.272023000
6	4.775758000	-1.239727000	0.661375000
1	4.595667000	-0.463149000	1.418728000
6	5.999513000	-1.919656000	0.637058000
1	6.775464000	-1.664093000	1.374943000
6	6.238577000	-2.924808000	-0.315593000
1	7.203386000	-3.454022000	-0.332998000
6	5.237528000	-3.247561000	-1.245150000
1	5.415568000	-4.027858000	-2.000939000
6	4.010115000	-2.570640000	-1.223903000
1	3.238977000	-2.809043000	-1.973814000
6	-2.574204000	-1.696374000	-1.622161000
6	-3.216111000	-1.771561000	1.183537000
6	-4.831479000	-0.287263000	-0.656229000
6	-3.269795000	1.099485000	1.281628000
6	-2.569968000	1.219800000	-1.534275000

2b_TS

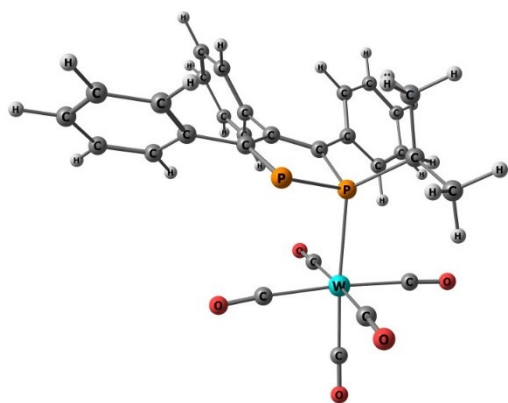


Charge : 0
 Multiplicity : 1
 Total energy: -18808.6746128868 a.u.

74	-2.119554966	-0.494996994	-0.826435955
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15	0.704551966	-1.717176006	0.430180955
8	-1.502455966	-3.324958994	-2.195143955
8	-4.044685966	-2.009294994	1.241203045
8	-4.416937966	-0.296501994	-2.957152955
8	-3.277712966	2.364189006	0.070656045
8	0.043640034	0.871448006	-2.758371955
6	0.761154966	1.022858994	0.907209955
6	2.017565966	0.588196994	0.384403955
6	2.202813966	-0.806621006	0.186041955
6	0.999300966	-3.319093006	1.373105955
1	1.727391966	-3.847509006	0.718876955
6	1.633700966	-3.073564006	2.746203955
1	0.954836966	-2.495181006	3.404900955
1	2.592279966	-2.524861006	2.666587955
1	1.837732966	-4.047650006	3.239805955
6	-0.300207034	-4.131463006	1.440378955
1	-0.105624034	-5.099117006	1.947057955
1	-0.709522034	-4.348870006	0.434715955
1	-1.083203034	-3.604937006	2.024212955
6	0.329408966	2.434666994	1.005708955

6	-0.355111034	2.890592994	2.160074955
1	-0.490349034	2.203575994	3.010253955
6	-0.838187034	4.203187994	2.240088955
1	-1.361185034	4.536980994	3.149133955
6	-0.655837034	5.087759994	1.165779955
1	-1.039332034	6.117676994	1.225308955
6	0.014755966	4.649227994	0.011597955
1	0.149798966	5.332508994	-0.840719045
6	0.506514966	3.340942994	-0.070267045
1	1.009166966	3.001607994	-0.986632045
6	3.091410966	1.564875994	0.026312955
6	3.592192966	2.469425994	0.988082955
1	3.180668966	2.454657994	2.008686955
6	4.606409966	3.378000994	0.652541955
1	4.988965966	4.073848994	1.414949955
6	5.129951966	3.402922994	-0.650124045
1	5.923243966	4.119064994	-0.913744045
6	4.634239966	2.511770994	-1.615664045
1	5.034332966	2.529755994	-2.641017045
6	3.626142966	1.596708994	-1.280641045
1	3.231623966	0.906396994	-2.041212045
6	3.428058966	-1.493619006	-0.261639045
6	4.686830966	-1.187079006	0.315785955
1	4.753637966	-0.396001006	1.076428955
6	5.836232966	-1.892112006	-0.061744045
1	6.801756966	-1.640970006	0.403626955
6	5.763865966	-2.914153006	-1.023448045
1	6.671194966	-3.461753006	-1.320055045
6	4.526148966	-3.226664006	-1.607271045
1	4.458321966	-4.016147006	-2.371354045
6	3.371681966	-2.524975006	-1.233339045
1	2.410078966	-2.749846006	-1.722226045
6	-1.672079966	-2.303804994	-1.656568955
6	-3.355113966	-1.446681994	0.491551045
6	-3.555843966	-0.381406994	-2.170422955
6	-2.803978966	1.340583006	-0.206597955
6	-0.752475966	0.388494006	-2.058171955

2b'



Charge : 0

Multiplicity : 1

Total energy: -18808.6881405080 a.u.

74	-1.476487000	-1.549899000	-1.506433000
15	-0.672515000	0.234485000	1.649484000
15	0.211110000	-1.384929000	0.456100000
8	-0.557053000	-4.571920000	-2.040756000
8	-3.789859000	-2.448078000	0.525955000
8	-3.486045000	-1.990607000	-3.905594000
8	-2.596988000	1.458884000	-1.374766000
8	0.734529000	-0.373643000	-3.505856000

6	0.623356000	1.303487000	1.182783000
6	1.777437000	0.799494000	0.431850000
6	1.795778000	-0.551706000	0.091104000
6	0.646444000	-2.895762000	1.499752000
1	1.225709000	-3.522053000	0.784912000
6	1.540972000	-2.525603000	2.687673000
1	1.006708000	-1.864353000	3.400122000
1	2.468924000	-2.012883000	2.368596000
1	1.834834000	-3.444892000	3.235803000
6	-0.611934000	-3.659291000	1.923273000
1	-0.320857000	-4.560046000	2.502020000
1	-1.209542000	-3.997443000	1.055640000
1	-1.267996000	-3.044140000	2.572952000
6	0.433662000	2.743676000	1.501253000
6	0.082694000	3.144083000	2.812902000
1	0.017773000	2.381966000	3.605302000
6	-0.159781000	4.491692000	3.114062000
1	-0.424143000	4.780937000	4.142698000
6	-0.060738000	5.467179000	2.109973000
1	-0.250770000	6.525547000	2.344975000
6	0.282311000	5.084280000	0.802427000
1	0.352370000	5.841262000	0.006375000
6	0.532140000	3.740097000	0.499476000
1	0.785854000	3.451002000	-0.530551000
6	2.888191000	1.720075000	0.044020000
6	3.562391000	2.501405000	1.008961000
1	3.264063000	2.434378000	2.065917000
6	4.611062000	3.352059000	0.631043000
1	5.131574000	3.948328000	1.396081000
6	4.992803000	3.448085000	-0.716937000
1	5.811912000	4.121216000	-1.012952000
6	4.321039000	2.685117000	-1.685906000
1	4.609077000	2.760077000	-2.745671000
6	3.279924000	1.824759000	-1.309989000
1	2.752586000	1.229666000	-2.071154000
6	2.938253000	-1.329349000	-0.429188000
6	4.257488000	-1.080774000	0.034031000
1	4.432692000	-0.275738000	0.761262000
6	5.334333000	-1.858541000	-0.406979000
1	6.345331000	-1.646943000	-0.026255000
6	5.131210000	-2.905376000	-1.321935000
1	5.980752000	-3.512735000	-1.669199000
6	3.833112000	-3.173575000	-1.782686000
1	3.656258000	-3.991209000	-2.497927000
6	2.751532000	-2.401101000	-1.338873000
1	1.743097000	-2.619243000	-1.717806000
6	-0.873109000	-3.472757000	-1.818677000
6	-2.932948000	-2.136480000	-0.196202000
6	-2.748826000	-1.815821000	-3.018713000
6	-2.169039000	0.379311000	-1.359324000
6	-0.056905000	-0.825593000	-2.781551000

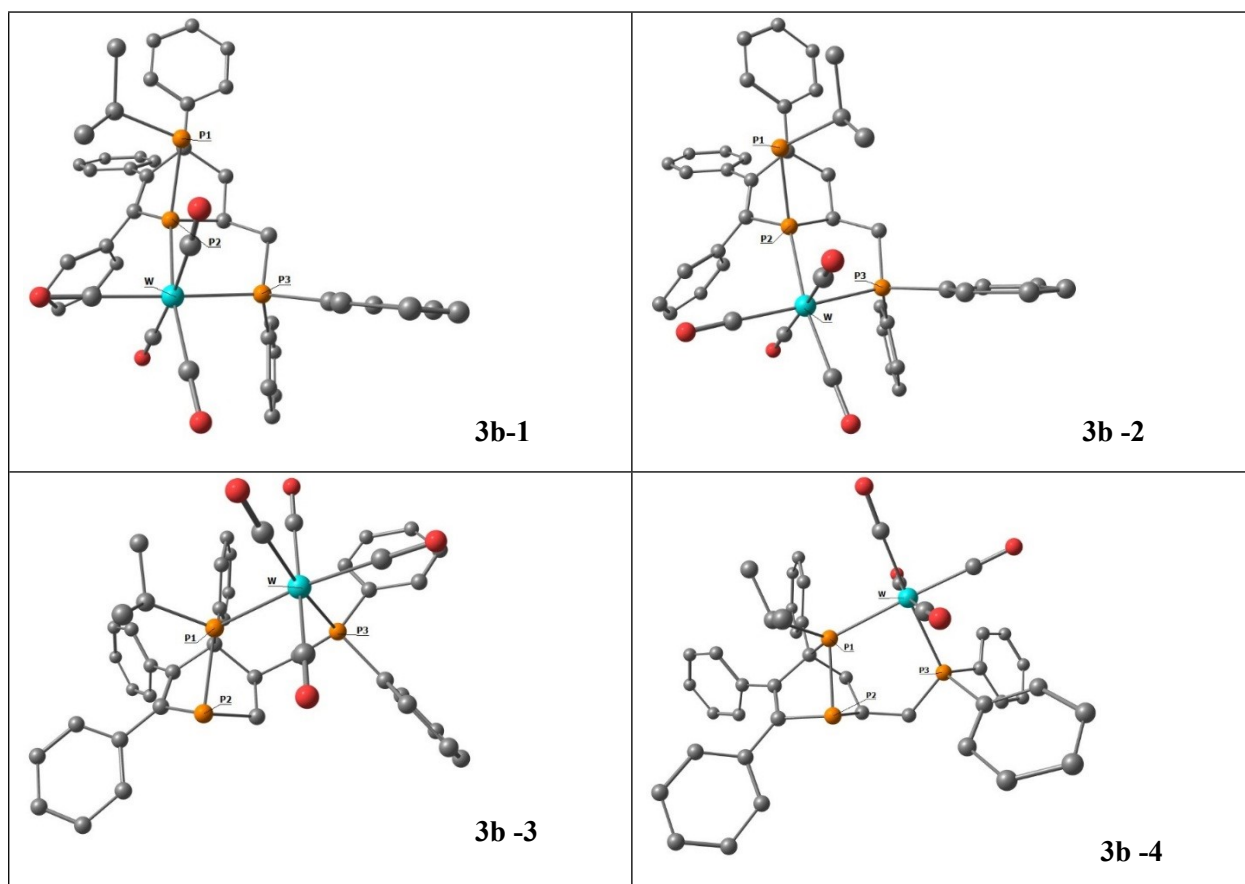
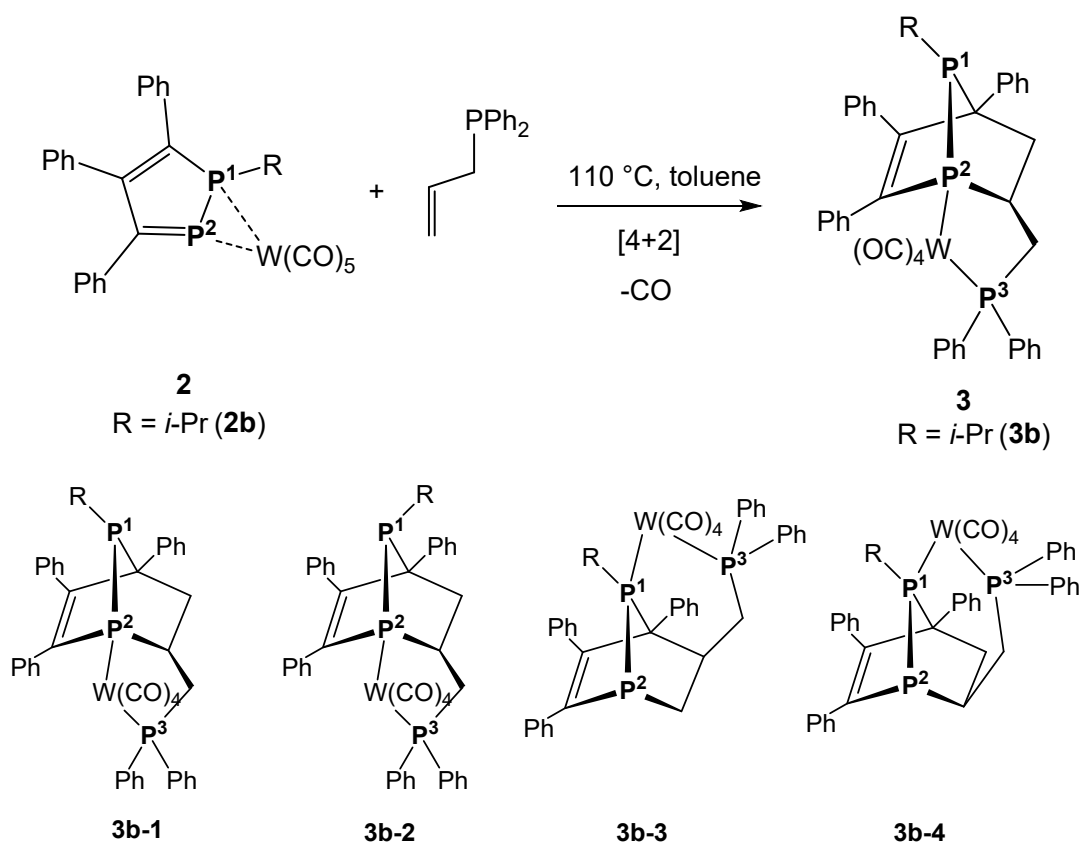


Figure S7. Optimized geometries of possible isomers of [4+2] cycloaddition reaction of complex **2b** with allyldiphenylphosphine. H atoms are omitted for clarity.

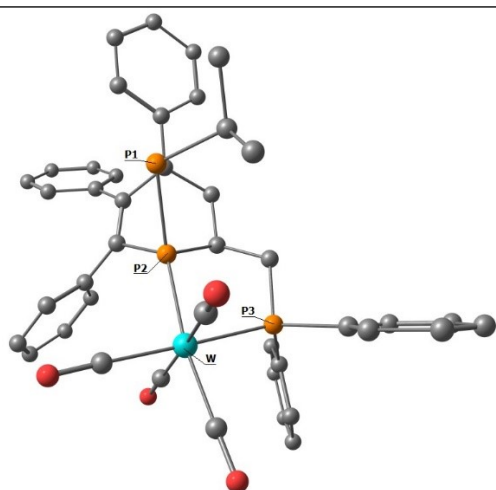
Table S3. Total and relative energies of possible isomers of **3b**

Compound	E_{Tot} , a.u.	E_{rel} , kcal/mol
3b-1	-19617.77306360	0.0
3b-2	-19617.77240139	0.42
3b-3	-19617.76296781	6.34
3b-4	-19617.76460584	5.31

Table S4. Cartesian coordinates and total energies of possible stereoisomers of complex **2b** with allyldiphenylphosphine

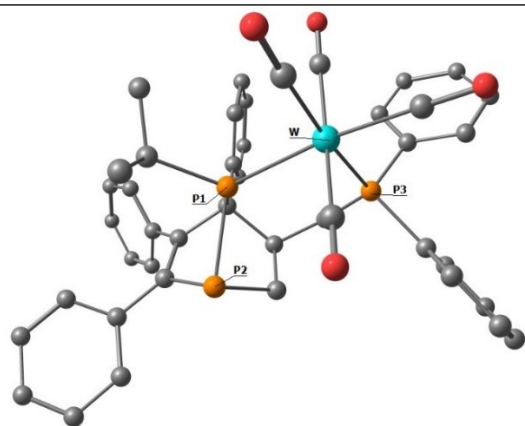
3b-1			
Charge : 0			
Multiplicity : 1			
Total energy: -19617.77306360 a.u.			
74	26.382229000	1.229597000	17.639615000
15	26.748998000	3.065588000	15.972243000
15	25.673831000	3.426725000	14.039955000
15	24.951905000	3.054061000	18.659630000
8	24.100866000	0.023904000	15.748705000
8	25.571517000	-0.746281000	19.972409000
8	28.883669000	2.157021000	19.417322000
8	28.331843000	-0.887786000	16.326783000
6	26.605599000	5.138878000	14.168410000
6	28.089358000	4.880259000	14.510441000
6	28.336474000	3.856950000	15.389049000
6	26.049828000	4.721173000	16.651149000
1	26.849765000	5.065462000	17.339885000
6	25.903116000	5.695617000	15.458629000
1	26.314742000	6.697118000	15.702872000
1	24.824835000	5.836625000	15.245302000
6	26.346291000	5.958070000	12.910943000
6	27.120262000	5.742739000	11.745773000
1	27.936757000	5.007215000	11.767284000
6	26.876883000	6.454819000	10.564231000
1	27.501068000	6.263745000	9.677876000
6	25.848852000	7.409684000	10.510749000
1	25.657806000	7.972248000	9.584352000
6	25.072265000	7.639606000	11.654614000
1	24.263523000	8.386236000	11.632910000
6	25.319583000	6.925581000	12.838301000
1	24.692588000	7.137316000	13.715144000
6	29.167621000	5.784416000	14.023411000
6	29.012404000	7.190604000	14.033949000
1	28.069369000	7.634045000	14.385226000
6	30.047155000	8.032249000	13.602622000
1	29.905929000	9.123652000	13.628833000
6	31.252898000	7.489105000	13.131612000
1	32.061492000	8.150647000	12.785211000
6	31.415266000	6.094519000	13.098538000
1	32.352477000	5.656188000	12.722639000
6	30.387300000	5.252389000	13.542212000
1	30.521687000	4.161134000	13.511728000
6	29.607862000	3.524928000	16.071856000

6	30.119562000	2.207263000	16.032419000
1	29.585136000	1.432417000	15.464309000
6	31.303563000	1.878592000	16.706974000
1	31.683522000	0.846671000	16.662698000
6	31.989782000	2.854944000	17.445919000
1	32.912176000	2.592829000	17.986222000
6	31.487944000	4.165473000	17.500954000
1	32.016191000	4.934751000	18.084859000
6	30.310361000	4.499435000	16.819452000
1	29.920007000	5.527222000	16.864403000
6	26.641468000	2.387856000	12.781815000
1	27.668930000	2.807826000	12.721895000
6	25.943957000	2.502203000	11.415786000
1	26.519322000	1.940512000	10.649409000
1	25.848575000	3.548432000	11.066369000
1	24.925279000	2.063776000	11.455499000
6	26.725701000	0.921575000	13.227677000
1	25.721140000	0.493040000	13.424775000
1	27.329862000	0.787460000	14.145539000
1	27.191806000	0.312209000	12.425055000
6	24.763733000	4.466931000	17.439615000
1	23.950597000	4.141009000	16.756662000
1	24.401223000	5.378503000	17.959963000
6	23.188238000	2.769411000	19.162955000
6	22.543831000	1.560084000	18.839289000
1	23.100237000	0.770467000	18.314745000
6	21.198619000	1.358704000	19.189410000
1	20.706827000	0.408184000	18.932597000
6	20.488806000	2.360701000	19.867326000
1	19.435322000	2.200715000	20.143717000
6	21.128568000	3.566425000	20.201522000
1	20.578569000	4.352235000	20.742042000
6	22.471940000	3.769755000	19.856060000
1	22.970729000	4.709055000	20.142250000
6	25.641618000	3.832479000	20.195109000
6	25.801582000	3.001929000	21.326879000
1	25.503840000	1.942949000	21.277894000
6	26.337385000	3.515660000	22.515121000
1	26.452535000	2.856363000	23.388921000
6	26.733225000	4.861859000	22.589360000
1	27.161069000	5.262096000	23.521079000
6	26.584988000	5.691328000	21.468899000
1	26.895157000	6.746543000	21.516889000
6	26.039517000	5.181431000	20.278035000
1	25.929725000	5.853461000	19.413959000
6	24.904722000	0.492054000	16.457051000
6	25.875582000	-0.025815000	19.099620000
6	27.968099000	1.856282000	18.763314000
6	27.607519000	-0.102330000	16.809280000
3b-2	Charge : 0 Multiplicity : 1 Total energy: -19617.77240139 a.u.		



74	26.448647000	1.401923000	17.807890000
15	26.721943000	3.245121000	16.112937000
15	25.958933000	3.588637000	14.020138000
15	24.998445000	3.212839000	18.836933000
8	24.276434000	-0.296800000	16.193028000
8	25.837911000	-0.467776000	20.280285000
8	28.971367000	2.452964000	19.479484000
8	28.444362000	-0.702991000	16.545581000
6	26.638231000	5.380545000	14.370162000
6	28.116636000	5.047315000	14.657808000
6	28.328119000	3.984918000	15.501093000
6	26.107337000	4.904681000	16.847968000
1	26.937178000	5.201401000	17.523982000
6	25.977478000	5.907771000	15.683376000
1	26.434967000	6.882870000	15.954633000
1	24.904425000	6.113696000	15.492453000
6	26.388773000	6.244542000	13.142470000
6	26.942877000	5.864445000	11.896676000
1	27.568402000	4.960901000	11.839682000
6	26.704447000	6.611626000	10.737338000
1	27.149573000	6.290355000	9.783212000
6	25.900951000	7.763451000	10.788530000
1	25.710322000	8.350455000	9.877267000
6	25.347418000	8.157211000	12.014175000
1	24.719090000	9.059389000	12.072635000
6	25.590804000	7.407909000	13.178283000
1	25.147373000	7.750092000	14.123827000
6	29.219392000	5.865913000	14.087154000
6	29.177469000	7.279263000	14.123639000
1	28.312591000	7.789357000	14.572534000
6	30.229585000	8.042855000	13.599288000
1	30.180199000	9.141583000	13.646242000
6	31.337066000	7.411893000	13.010851000
1	32.159060000	8.012386000	12.592106000
6	31.384905000	6.009597000	12.953994000
1	32.244242000	5.504499000	12.486880000
6	30.340226000	5.244452000	13.489036000
1	30.380890000	4.146702000	13.438841000
6	29.621008000	3.543856000	16.073571000
6	30.059295000	2.209303000	15.920515000
1	29.450022000	1.500043000	15.342497000
6	31.266457000	1.783083000	16.491567000
1	31.585807000	0.737740000	16.363252000

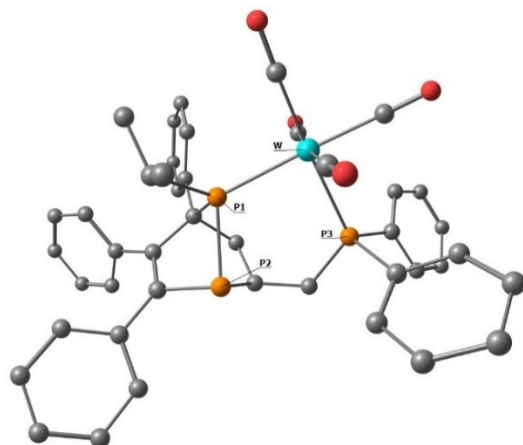
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6	30.424699000	4.438611000	16.817701000
1	30.092279000	5.479499000	16.948689000
6	24.066008000	3.783605000	14.037976000
6	24.837736000	4.680845000	17.672252000
1	23.981997000	4.421740000	17.015210000
1	24.538361000	5.585253000	18.242653000
6	23.222632000	2.933377000	19.300324000
6	22.555580000	1.769902000	18.871819000
1	23.103133000	1.011106000	18.294971000
6	21.199706000	1.575331000	19.183275000
1	20.690408000	0.659699000	18.846120000
6	20.502139000	2.538752000	19.926813000
1	19.440803000	2.383496000	20.174398000
6	21.163894000	3.699066000	20.363550000
1	20.622661000	4.453987000	20.954618000
6	22.517750000	3.895547000	20.056458000
1	23.033928000	4.797924000	20.419866000
6	25.673232000	3.929288000	20.408473000
6	25.708027000	3.092661000	21.546568000
1	25.316702000	2.065278000	21.487859000
6	26.240518000	3.560023000	22.755420000
1	26.257588000	2.896729000	23.633638000
6	26.756451000	4.863879000	22.845445000
1	27.180126000	5.227199000	23.794032000
6	26.734107000	5.697487000	21.718571000
1	27.140155000	6.719046000	21.777900000
6	26.194148000	5.234760000	20.506271000
1	26.189733000	5.909216000	19.636995000
6	25.024000000	0.392081000	16.771980000
6	26.067807000	0.211353000	19.353209000
6	28.043595000	2.123765000	18.857003000
6	27.710557000	0.087818000	17.000313000
6	23.617002000	4.076393000	12.595679000
1	23.882631000	3.238131000	11.918330000
1	22.512985000	4.195892000	12.561466000
1	24.069549000	5.000261000	12.185271000
6	23.385264000	2.523877000	14.585497000
1	22.285755000	2.594368000	14.446110000
1	23.725219000	1.606384000	14.062279000
1	23.577510000	2.375445000	15.665186000
1	23.791613000	4.649202000	14.677898000
3b-3	Charge : 0 Multiplicity : 1 Total energy: -19617.76296781 a.u.		



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6	-3.750654000	-1.819894000	0.750083000
6	-3.971006000	-0.888850000	-0.235071000
6	-3.349944000	-1.446081000	2.137077000
6	-4.149703000	-1.786183000	3.252681000
6	-2.158348000	-0.719720000	2.361655000
6	-3.774662000	-1.401692000	4.547623000
1	-5.079357000	-2.354272000	3.100347000
6	-1.777640000	-0.347232000	3.658961000
1	-1.529668000	-0.442064000	1.502003000
6	-2.585484000	-0.684503000	4.756641000
1	-4.415910000	-1.668963000	5.401493000
1	-0.843611000	0.214876000	3.812657000
1	-2.288844000	-0.388968000	5.774616000
6	-3.962441000	0.587276000	-0.109321000
6	-3.448751000	1.384029000	-1.161825000
6	-4.504298000	1.252259000	1.018667000
6	-3.445888000	2.783135000	-1.079082000
1	-3.042217000	0.893813000	-2.060760000
6	-4.512405000	2.650935000	1.094238000
1	-4.935695000	0.662297000	1.839590000
6	-3.976949000	3.424288000	0.050980000
1	-3.031486000	3.376690000	-1.908439000
1	-4.947847000	3.142962000	1.977644000
1	-3.983446000	4.523121000	0.114371000
6	-3.794308000	-4.310198000	1.464804000
6	-2.620043000	-4.416220000	2.250623000
6	-4.849464000	-5.193197000	1.758624000
6	-2.517187000	-5.357904000	3.283224000
1	-1.768966000	-3.745621000	2.061095000
6	-4.753123000	-6.142067000	2.791469000
1	-5.765896000	-5.160084000	1.158469000
6	-3.585632000	-6.227293000	3.561344000
1	-1.592479000	-5.410581000	3.878180000
1	-5.598692000	-6.821215000	2.977685000
1	-3.504303000	-6.967841000	4.371648000
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15	-5.406329000	-3.355620000	-0.858673000
6	-6.837647000	-2.439661000	-0.000797000
6	-7.676468000	-3.329051000	0.925373000
6	-7.716403000	-1.770398000	-1.069912000
1	-6.347995000	-1.645711000	0.600236000
1	-7.120851000	-3.651315000	1.826415000
1	-8.565322000	-2.760918000	1.270885000
1	-8.048250000	-4.233199000	0.401767000

1	-7.139646000	-1.098400000	-1.736178000
1	-8.237128000	-2.516609000	-1.700800000
1	-8.496256000	-1.159108000	-0.569626000
15	-3.425747000	-5.955285000	-2.216908000
6	-2.396398000	-5.906736000	-3.772913000
6	-2.954659000	-5.484004000	-4.993125000
6	-1.042426000	-6.311829000	-3.746901000
6	-2.174576000	-5.446209000	-6.161670000
1	-4.009467000	-5.179773000	-5.027549000
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1	-0.590788000	-6.678652000	-2.811616000
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6	-3.127472000	-9.442421000	0.041626000
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6	-3.020259000	-10.086347000	-2.293621000
1	-3.094396000	-8.474758000	-3.739578000
6	-3.029038000	-10.443577000	-0.936393000
1	-3.148106000	-9.709839000	1.109258000
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74	-5.904359000	-5.356688000	-2.341361000
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1	-2.319554000	-5.616600000	-0.061000000
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1	-1.965230000	-2.011379000	-2.144321000
1	-2.901694000	-3.323914000	-2.889880000
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3b-4



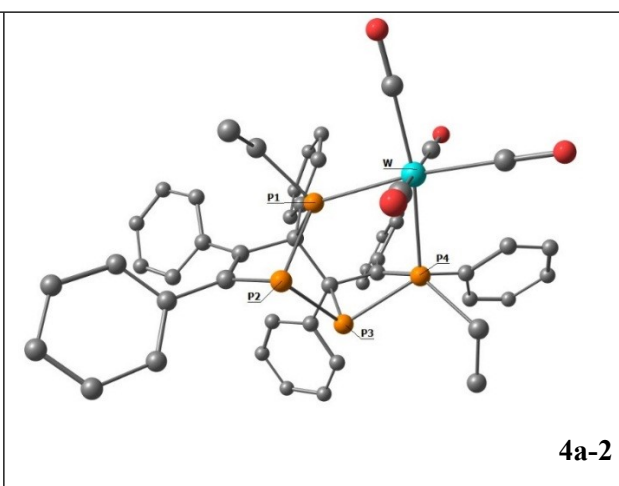
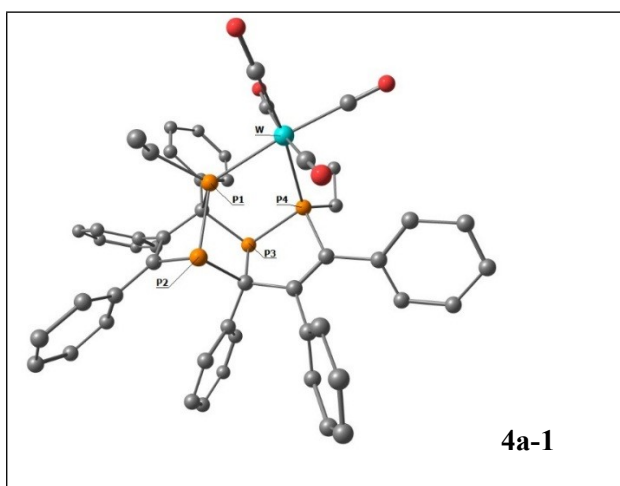
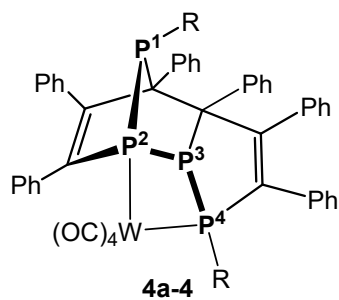
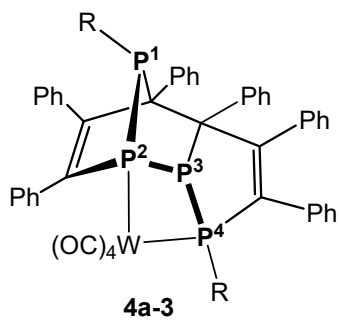
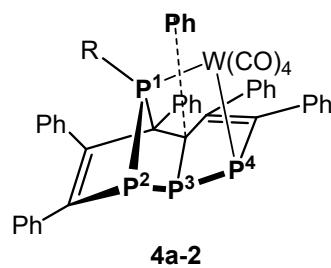
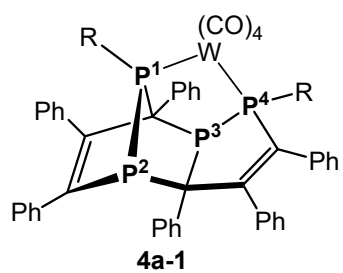
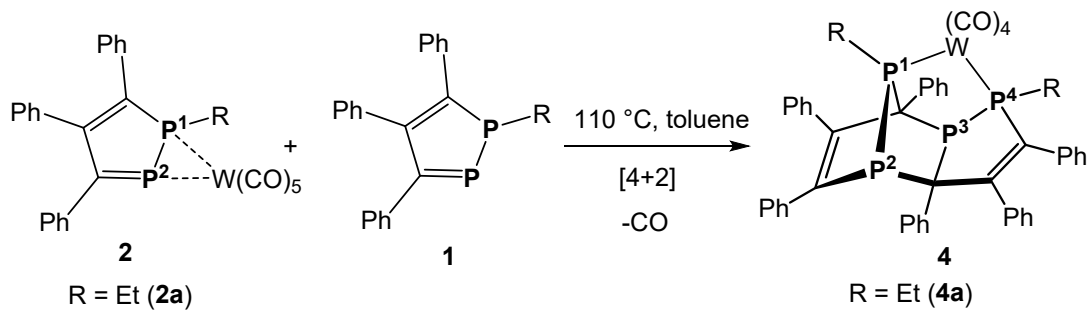
Charge : 0

Multiplicity : 1

Total energy: -19617.76460584 a.u.

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6	2.599991000	-4.349824000	-1.463374000
6	3.621819000	-5.195165000	-1.953311000
6	2.945348000	-3.035449000	-1.073219000
6	4.946823000	-4.744066000	-2.034791000
1	3.375672000	-6.220117000	-2.267017000
6	4.268410000	-2.581368000	-1.167922000
1	2.159664000	-2.367408000	-0.689011000
6	5.275188000	-3.435312000	-1.646078000
1	5.728933000	-5.420982000	-2.411232000
1	4.514754000	-1.552748000	-0.862653000
1	6.314786000	-3.080783000	-1.717781000
6	1.025105000	-4.497512000	1.196437000
6	0.213895000	-3.806490000	2.129503000
6	2.311680000	-4.913573000	1.620964000
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1	1.835891000	-9.506457000	-1.354821000
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6	-6.022414000	-6.042412000	0.909628000
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6	-2.084843000	-6.658108000	-5.123954000
8	-1.364923000	-10.173843000	-4.192610000
8	-5.345150000	-8.454795000	-4.887271000
8	-1.744523000	-6.275225000	-6.174201000
6	-1.680228000	-3.965711000	-1.613237000
1	-1.413725000	-3.038868000	-1.063237000
6	-3.166910000	-3.838382000	-1.980750000
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1	-7.290678000	-2.596925000	-6.627152000
74	-2.754198000	-7.457051000	-3.375544000
6	-3.514061000	-8.387617000	-1.730058000
8	-3.987278000	-8.969054000	-0.837358000



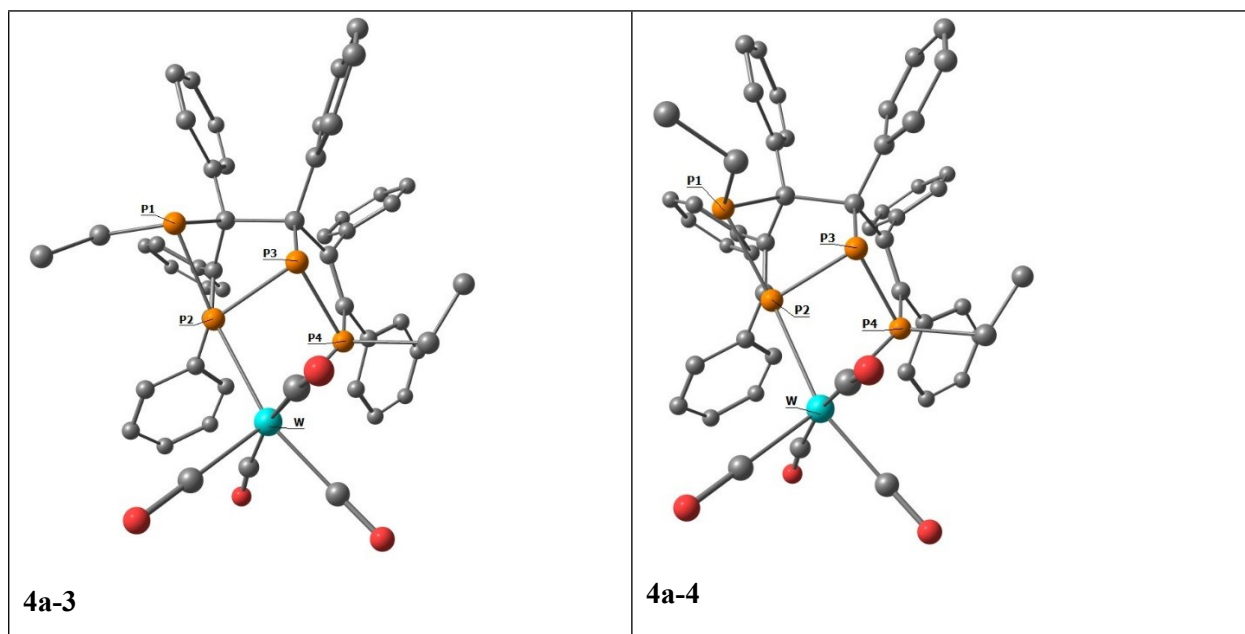


Figure S8. Optimized geometries of possible isomers of complex **4a**. H atoms are omitted for clarity.

Table S5. Total and relative energies of possible isomers of **4a**

Compound	E_{Tot} , a.u.	E_{rel} , kcal/mol
4a-1	-20228.46764892	0.0
4a-2	-20228.44273605	15.63
4a-3	-20228.391907617	47.53
4a-4	-20228.388520814	49.65

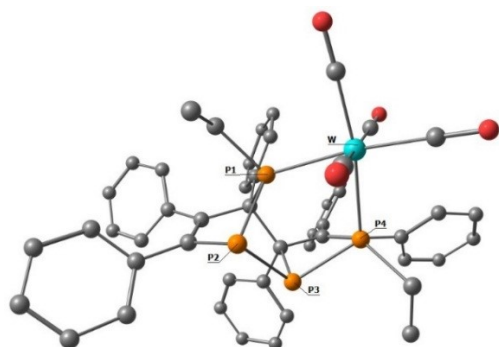
Table S6. Cartesian coordinates and total energies of possible stereoisomers of **4a**.

4a-1			
Charge : 0			
Multiplicity : 1			
Total energy: -20228.46764892 a.u.			
74	2.887107000	0.277547000	12.424804000
15	1.204940000	1.564556000	13.794822000
15	-0.953394000	1.058191000	13.335056000
15	0.760141000	-0.154160000	11.191415000
15	-0.480978000	1.475177000	10.235107000
8	3.578248000	2.715576000	10.474825000
8	5.399399000	1.022257000	14.204540000
8	4.649930000	-1.483868000	10.479887000
8	2.764160000	-2.425752000	14.139102000
6	0.937239000	3.311132000	13.236633000
6	-0.040565000	3.498024000	12.295475000
6	-1.005774000	2.356192000	11.928050000
6	-0.796033000	-0.545837000	12.273198000
6	-1.973733000	-0.579455000	11.293196000
6	-1.948481000	0.309755000	10.244816000
6	1.275583000	1.703224000	15.663966000
1	1.867490000	2.624572000	15.847779000
1	0.244525000	1.908591000	16.020461000
6	1.907343000	0.510654000	16.379547000
1	1.371315000	-0.438116000	16.181543000
1	1.902123000	0.679258000	17.475674000
1	2.960423000	0.367158000	16.067886000
6	1.824208000	4.372774000	13.781965000
6	3.225533000	4.202777000	13.879267000
1	3.684974000	3.279972000	13.499964000
6	4.034800000	5.199189000	14.443304000
1	5.122881000	5.042431000	14.498255000
6	3.463959000	6.384082000	14.932622000
1	4.100073000	7.165320000	15.376111000
6	2.072679000	6.560392000	14.859264000
1	1.610595000	7.479978000	15.250379000
6	1.261774000	5.566789000	14.295270000
1	0.172351000	5.707355000	14.257276000
6	-0.126532000	4.791949000	11.541723000
6	0.867903000	5.088592000	10.582500000
1	1.679680000	4.368411000	10.404180000
6	0.833826000	6.295029000	9.866596000
1	1.617886000	6.506503000	9.123479000

6	-0.186198000	7.229051000	10.102557000
1	-0.209115000	8.178045000	9.544963000
6	-1.175060000	6.948540000	11.059124000
1	-1.975594000	7.677813000	11.257463000
6	-1.150804000	5.738797000	11.767860000
1	-1.930987000	5.529310000	12.514393000
6	-2.434902000	2.901824000	11.739345000
6	-2.838045000	3.465624000	10.508197000
1	-2.139833000	3.471804000	9.656981000
6	-4.111462000	4.028847000	10.347167000
1	-4.396030000	4.450470000	9.371366000
6	-5.015125000	4.054357000	11.420026000
1	-6.015886000	4.495483000	11.294935000
6	-4.629356000	3.508504000	12.653499000
1	-5.324939000	3.520884000	13.506928000
6	-3.354783000	2.940042000	12.809732000
1	-3.069072000	2.517533000	13.784903000
6	0.806317000	-1.399814000	9.789224000
1	1.301734000	-2.293710000	10.220317000
1	-0.232502000	-1.674811000	9.517316000
6	1.581642000	-0.900321000	8.565832000
1	1.102152000	-0.012789000	8.105583000
1	1.625312000	-1.697685000	7.796052000
1	2.624243000	-0.628987000	8.819850000
6	-0.620746000	-1.790032000	13.133967000
6	-0.631699000	-1.746199000	14.543866000
1	-0.809929000	-0.788396000	15.057040000
6	-0.449241000	-2.905660000	15.313637000
1	-0.459242000	-2.834714000	16.412096000
6	-0.257043000	-4.144280000	14.688195000
1	-0.107949000	-5.054362000	15.288523000
6	-0.264202000	-4.212140000	13.286074000
1	-0.127743000	-5.179549000	12.779156000
6	-0.447127000	-3.053151000	12.521462000
1	-0.472829000	-3.137647000	11.426435000
6	-3.067520000	-1.569301000	11.507180000
6	-3.762400000	-1.628159000	12.736500000
1	-3.495225000	-0.930470000	13.544812000
6	-4.795681000	-2.555855000	12.930078000
1	-5.330627000	-2.581188000	13.891851000
6	-5.143347000	-3.452448000	11.906971000
1	-5.948939000	-4.185999000	12.063500000
6	-4.452324000	-3.411388000	10.685263000
1	-4.713269000	-4.114249000	9.879150000
6	-3.427056000	-2.476884000	10.485583000
1	-2.891456000	-2.446783000	9.524550000
6	-2.986466000	0.488891000	9.202177000
6	-4.367949000	0.504838000	9.513238000
1	-4.686478000	0.394912000	10.559291000
6	-5.326228000	0.689067000	8.509227000
1	-6.394099000	0.706993000	8.776378000
6	-4.932703000	0.861542000	7.171241000
1	-5.689007000	1.005357000	6.384390000
6	-3.566838000	0.861340000	6.847724000
1	-3.244901000	1.002687000	5.804512000
6	-2.605054000	0.686127000	7.852946000
1	-1.535240000	0.696034000	7.591389000
6	3.292323000	1.851298000	11.207420000

6	4.472942000	0.743441000	13.544625000
6	4.001936000	-0.823829000	11.199188000
6	2.726049000	-1.426879000	13.538818000

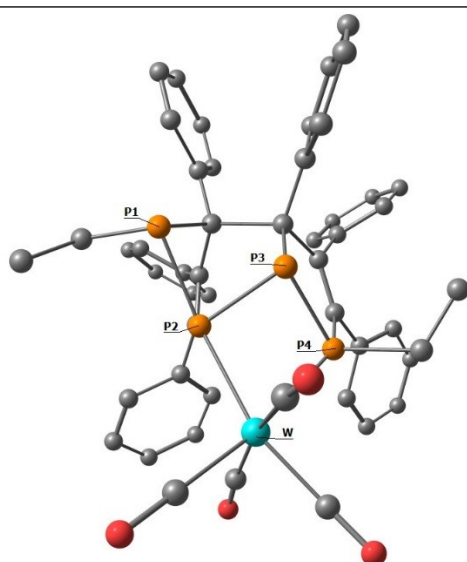
4a-2



Charge : 0
 Multiplicity : 1
 Total energy: -20228.44273605 a.u.

6	-3.476097000	0.088292000	0.212043000
6	-3.588395000	1.457446000	0.272746000
15	-0.864119000	0.292319000	-1.486439000
15	1.142948000	0.935902000	-0.702631000
6	-4.562634000	-0.922684000	0.316298000
6	-4.657089000	-1.956161000	-0.644125000
6	-5.468658000	-0.929854000	1.402674000
6	-5.645287000	-2.945705000	-0.540026000
1	-3.949714000	-1.974751000	-1.488438000
6	-6.446566000	-1.927829000	1.511776000
1	-5.399050000	-0.144434000	2.169605000
6	-6.543952000	-2.935627000	0.538491000
1	-5.707994000	-3.734728000	-1.305039000
1	-7.137814000	-1.919735000	2.368521000
1	-7.313527000	-3.717700000	0.625553000
6	-4.931571000	2.082284000	0.509684000
6	-5.162674000	2.960338000	1.595938000
6	-6.041640000	1.728897000	-0.297740000
6	-6.447395000	3.458279000	1.862519000
1	-4.332062000	3.257798000	2.249910000
6	-7.320948000	2.236140000	-0.037201000
1	-5.892135000	1.043763000	-1.144395000
6	-7.531656000	3.103803000	1.046680000
1	-6.596043000	4.134546000	2.718155000
1	-8.161810000	1.945317000	-0.685417000
1	-8.536880000	3.501478000	1.253777000
6	-2.346193000	3.731430000	0.647218000
6	-3.148341000	4.685562000	-0.022325000
6	-1.635394000	4.183544000	1.779015000
6	-3.248634000	6.007113000	0.431203000
1	-3.704150000	4.407286000	-0.924234000
6	-1.730375000	5.505981000	2.241005000
1	-0.961804000	3.498654000	2.314232000
6	-2.546474000	6.426140000	1.571378000
1	-3.880848000	6.717522000	-0.122338000
1	-1.150892000	5.810857000	3.125491000
1	-2.626021000	7.464878000	1.926508000
6	-2.168361000	1.135141000	3.029462000
6	-2.100445000	-0.218717000	3.740123000
1	-3.216422000	1.399025000	2.790075000
1	-1.765298000	1.934583000	3.683228000
1	-2.621051000	-0.157987000	4.717458000
1	-2.589180000	-1.018559000	3.148174000

1	-1.057468000	-0.533157000	3.940359000
6	2.374506000	-0.033551000	-1.715822000
6	2.171432000	-0.068006000	-3.228358000
1	2.354070000	-1.050489000	-1.269212000
1	3.361539000	0.395895000	-1.443397000
1	2.955196000	-0.688899000	-3.708283000
1	1.187206000	-0.500181000	-3.499361000
1	2.233937000	0.947242000	-3.668578000
6	-2.256073000	2.268377000	0.185423000
6	-0.361371000	3.071417000	-1.546942000
6	0.925366000	2.586467000	-1.509807000
6	-1.564846000	2.109941000	-1.296666000
6	2.144796000	3.290043000	-1.987998000
6	3.363267000	3.252530000	-1.268501000
6	2.135186000	3.952015000	-3.241463000
6	4.517571000	3.871295000	-1.769720000
1	3.401854000	2.742661000	-0.295111000
6	3.290280000	4.565616000	-3.741246000
1	1.206021000	3.979037000	-3.828638000
6	4.487266000	4.533287000	-3.006257000
1	5.447817000	3.834902000	-1.182545000
1	3.254896000	5.072913000	-4.717672000
1	5.393726000	5.018394000	-3.399275000
6	-0.578986000	4.535182000	-1.819063000
6	0.095295000	5.463189000	-0.986510000
6	-1.367076000	5.054957000	-2.874487000
6	-0.025791000	6.843509000	-1.185414000
1	0.712624000	5.091644000	-0.158146000
6	-1.480901000	6.439335000	-3.074977000
1	-1.879664000	4.381463000	-3.570611000
6	-0.817308000	7.342169000	-2.231720000
1	0.504555000	7.533682000	-0.511665000
1	-2.092707000	6.811567000	-3.911427000
1	-0.911125000	8.427240000	-2.392536000
6	-2.472826000	2.194550000	-2.554299000
6	-1.872416000	1.896765000	-3.807435000
6	-3.830551000	2.557867000	-2.580574000
6	-2.587338000	1.967208000	-5.008333000
1	-0.808259000	1.619982000	-3.845880000
6	-4.557915000	2.625266000	-3.782817000
1	-4.358102000	2.801938000	-1.656151000
6	-3.944097000	2.333076000	-5.005989000
1	-2.077001000	1.732654000	-5.955020000
1	-5.619875000	2.913801000	-3.746982000
1	-4.512025000	2.386628000	-5.947111000
15	-1.753718000	-0.623545000	0.347509000
15	-1.138156000	1.204365000	1.457887000
74	1.361650000	1.142682000	1.790393000
6	3.340575000	0.904842000	1.853931000
6	1.264501000	-0.876148000	2.060276000
6	1.197495000	1.327566000	3.765276000
6	1.691642000	3.145795000	1.772479000
8	1.286264000	-2.019660000	2.291234000
8	4.502760000	0.763391000	1.871474000
8	1.068560000	1.435993000	4.924897000
8	1.941479000	4.284974000	1.853053000
4a-3			Charge : 0 Multiplicity : 1

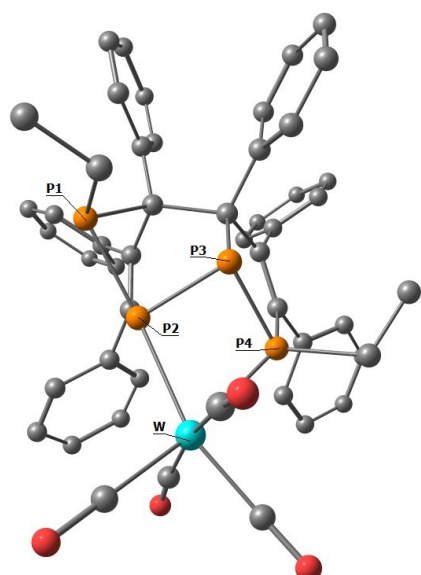


Total energy: -20228.391907617 a.u.

6	-3.603313000	0.198870000	-0.163699000
6	-3.662042000	1.550187000	-0.388028000
15	-1.315766000	1.565676000	1.157445000
15	-0.376181000	0.301272000	-1.161046000
15	-1.251506000	-1.212881000	-2.458045000
6	-4.752378000	-0.724779000	0.025450000
6	-5.607262000	-1.124892000	-1.025002000
6	-5.011002000	-1.227461000	1.323786000
6	-6.698748000	-1.970282000	-0.781959000
6	-6.105317000	-2.067974000	1.567014000
6	-6.956384000	-2.439303000	0.514352000
6	-5.000150000	2.231099000	-0.398756000
6	-5.353108000	3.091790000	0.669214000
6	-5.980224000	1.975401000	-1.382905000
6	-6.626990000	3.670084000	0.744800000
6	-7.252742000	2.565458000	-1.316377000
6	-7.582390000	3.416308000	-0.252179000
6	-2.399902000	3.817290000	-0.243285000
6	-3.324012000	4.597880000	-0.977681000
6	-1.513351000	4.512000000	0.609654000
6	-3.377405000	5.991692000	-0.840572000
6	-1.561565000	5.906926000	0.752872000
6	-2.501819000	6.655993000	0.031910000
6	-2.511942000	1.809895000	2.585078000
6	-2.062798000	1.011703000	3.813712000
6	-2.313308000	2.297688000	-0.389344000
6	-2.136306000	1.383943000	-3.019833000
6	-2.331848000	0.047606000	-3.320351000
6	-1.333544000	1.849514000	-1.768787000
15	-1.917050000	-0.432596000	0.305863000
74	-1.374784000	-2.853534000	-0.439587000
6	-0.950566000	-4.436037000	-1.530780000
6	-3.280430000	-3.556636000	-0.589086000
6	-1.290578000	-3.821191000	1.288213000
6	0.633017000	-2.615471000	-0.235464000
8	-1.243513000	-4.390204000	2.310134000
8	-0.691512000	-5.367451000	-2.194494000
8	1.794413000	-2.612955000	-0.111123000
8	-4.286451000	-4.141753000	-0.679042000
6	-3.170808000	-0.558512000	-4.399022000
6	-3.338348000	-0.033386000	-5.705480000

6	-3.810930000	-1.793665000	-4.109195000
6	-4.122189000	-0.702204000	-6.656845000
6	-4.605110000	-2.451870000	-5.057539000
6	-4.768000000	-1.907069000	-6.340272000
6	-2.614542000	2.400158000	-4.023795000
6	-1.706001000	2.824578000	-5.024893000
6	-3.928427000	2.903589000	-4.066443000
6	-2.099342000	3.726912000	-6.022569000
6	-4.324138000	3.808177000	-5.066464000
6	-3.412770000	4.225496000	-6.046928000
6	-0.311397000	2.980876000	-2.052161000
6	1.058803000	2.831030000	-1.730466000
6	-0.688239000	4.225721000	-2.615345000
6	1.998593000	3.847569000	-1.964832000
6	0.244997000	5.244791000	-2.851458000
6	1.598082000	5.064219000	-2.531041000
6	-0.046326000	-1.655175000	-3.819357000
6	0.552416000	-0.518996000	-4.641971000

4a-4



Charge : 0
 Multiplicity : 1
 Total energy: -20228.388520814 a.u.

6	-3.549319000	0.334708000	-0.222661000
6	-3.598361000	1.697691000	-0.385357000
15	-1.646801000	1.702574000	1.321367000
15	-0.303903000	0.397995000	-1.099398000
15	-1.047531000	-1.185735000	-2.391792000
6	-4.711842000	-0.570791000	-0.050822000
6	-5.571820000	-0.891843000	-1.124859000
6	-4.977488000	-1.141194000	1.216880000
6	-6.671100000	-1.741021000	-0.934769000
1	-5.357088000	-0.490784000	-2.125813000
6	-6.080941000	-1.983311000	1.406181000
1	-4.318400000	-0.904171000	2.066324000
6	-6.931703000	-2.286229000	0.331067000
1	-7.322782000	-1.986042000	-1.787336000
1	-6.274972000	-2.409699000	2.402066000
1	-7.791983000	-2.956514000	0.478701000
6	-4.889554000	2.427202000	-0.132005000
6	-4.976224000	3.227765000	1.034718000
6	-6.055710000	2.284238000	-0.913229000
6	-6.168672000	3.871613000	1.386051000
1	-4.092987000	3.327943000	1.682258000

6	-7.249911000	2.936438000	-0.565849000
1	-6.046096000	1.644482000	-1.803899000
6	-7.311960000	3.738132000	0.581746000
1	-6.203699000	4.480574000	2.302356000
1	-8.140794000	2.804685000	-1.198902000
1	-8.248648000	4.247230000	0.855474000
6	-2.325838000	3.936531000	-0.372090000
6	-3.282011000	4.657406000	-1.125978000
6	-1.456983000	4.685589000	0.447894000
6	-3.370923000	6.053594000	-1.051071000
1	-3.966281000	4.122595000	-1.797213000
6	-1.541407000	6.084963000	0.529280000
1	-0.681195000	4.178141000	1.036099000
6	-2.502792000	6.777632000	-0.218440000
1	-4.130153000	6.578172000	-1.651057000
1	-0.845085000	6.632169000	1.182804000
1	-2.575296000	7.874148000	-0.155220000
6	0.221304000	1.874953000	1.623672000
6	0.501558000	2.537504000	2.978464000
1	0.711570000	2.422096000	0.793107000
1	0.646479000	0.848710000	1.599090000
1	1.592247000	2.572334000	3.178003000
1	0.121002000	3.578818000	3.022953000
1	0.025655000	1.980641000	3.810892000
6	-2.227583000	2.414171000	-0.454219000
6	-2.070583000	1.350691000	-3.012914000
6	-2.145231000	0.006436000	-3.313366000
6	-1.270104000	1.898423000	-1.784678000
15	-1.878661000	-0.314321000	0.279339000
74	-1.321150000	-2.756934000	-0.341551000
6	-0.818433000	-4.362744000	-1.367595000
6	-3.223207000	-3.425627000	-0.638502000
6	-1.383689000	-3.698042000	1.404402000
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8	-1.421682000	-4.254876000	2.432865000
8	-0.508237000	-5.305377000	-1.991602000
8	1.810858000	-2.480916000	0.232067000
8	-4.237137000	-3.976231000	-0.812579000
6	-2.910826000	-0.643104000	-4.420025000
6	-2.862097000	-0.216605000	-5.768859000
6	-3.667992000	-1.804893000	-4.122793000
1	-2.267271000	0.663771000	-6.044126000
1	-3.706594000	-2.175055000	-3.087953000
6	-3.559835000	-0.909150000	-6.768866000
6	-4.374752000	-2.487743000	-5.122603000
1	-3.499342000	-0.556982000	-7.810192000
1	-4.960899000	-3.380059000	-4.854863000
6	-4.325580000	-2.042067000	-6.452392000
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6	-1.996538000	2.930225000	-4.988364000
6	-4.135575000	2.520632000	-3.931849000
1	-0.913818000	2.750100000	-5.053526000
1	-4.736744000	2.014978000	-3.167154000
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6	-4.004786000	3.990418000	-5.866089000
1	-4.493363000	4.646138000	-6.602861000
6	-0.242506000	2.992936000	-2.194257000
6	1.150551000	2.780563000	-2.056944000
6	-0.628656000	4.242375000	-2.739017000
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1	-1.685821000	4.478893000	-2.883130000
6	2.099612000	3.747386000	-2.426749000
6	0.312404000	5.214323000	-3.107733000
1	3.170439000	3.527901000	-2.296333000
1	-0.043236000	6.170762000	-3.520800000
6	1.685666000	4.977358000	-2.953389000
1	2.423546000	5.741913000	-3.240888000
6	0.205252000	-1.645682000	-3.701282000
6	0.849623000	-0.512884000	-4.493710000
1	0.957369000	-2.246266000	-3.148736000
1	-0.330374000	-2.358720000	-4.364842000
1	1.583396000	-0.918046000	-5.220182000
1	1.389585000	0.195630000	-3.833179000
1	0.098316000	0.067218000	-5.064844000