Supplementary Information

Solid-State ^{11}B NMR Studies of Coinage Metal Complexes Containing a Phosphine Substituted Diboraantracene Ligand

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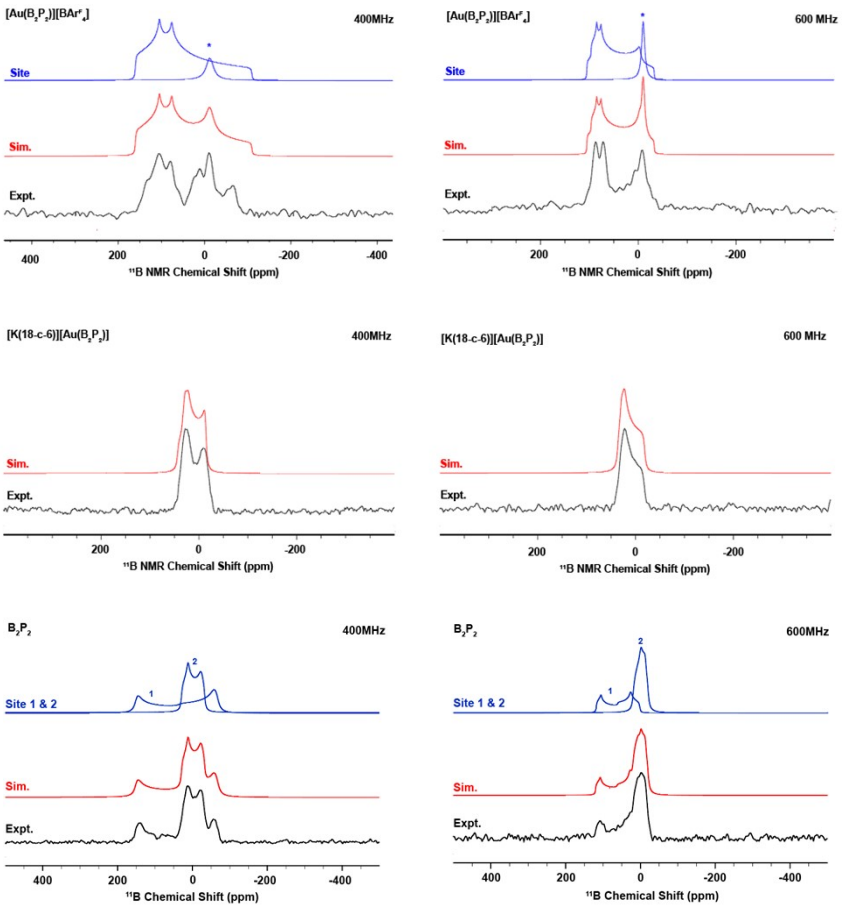


Figure S1. Solid-state ^{11}B NMR simulations at 400 and 600 MHz. * refers to $[\mathbf{B}Ar^{F}_{4}]^{-}$.

Table S1. Experimental ^{11}B NMR Parameters of B_2P_2 compounds.

chemical shift (ppm)	**$[Cu(B_2P_2)]^+$ $[PF_6]^-$**	**$[Cu(B_2P_2)]^+$ $[BAr^F{}_4]^-$**	**$[Ag(B_2P_2)]^+$ $[BAr^F{}_4]^-$**	**$[Au(B_2P_2)]^+$ $[BAr^F{}_4]^-$**	**$[Au(B_2P_2)]^-$ $[K(18\text{-c-}6)]^+$**	**B_2P_2**
$\delta(^{11}B)_{solution}$	27 (CD_3CN)	47 ($CDCl_3$)	29 (CD_3CN)	32 ($CDCl_3$)	11 (C_6D_6)	34 (C_6D_6)

Table S2. Simulated parameters for solid-state ^{11}B NMR (400MHz) of B_2P_2 compounds.
(* $[BAr^F{}_4]^-$ signal provided in parentheses, simulated with only chemical shift.)

Compounds	**δ_{iso}* (ppm)**	**Ω (ppm)**	**κ**	**C_Q (MHz)**	**η**	**α (deg.)**	**β (deg.)**	**γ (deg.)**
$[Cu(B_2P_2)]^+[PF_6]^-$	53	92	0.27	4.36	0.2	180	0	90
$[Ag(B_2P_2)]^+[BAr^F{}_4]^-$	57(-12)	102	0.39	4.49	0.04	280	180	92
$[Au(B_2P_2)]^+[BAr^F{}_4]^-$	70 (-11)	145	0.16	4.52	0.02	173	123	38
$[Au(B_2P_2)]^-[K(18\text{-c-}6)]^+$	17	56	0.73	1.51	0.21	60	90	180
B_2P_2 Site 1	65	74	0.71	4.68	0.08	124	4	274
B_2P_2 Site 2	9	36	-0.16	2.85	0.013	15	175	200

Table S3. Simulated parameters for solid-state ^{11}B NMR (600MHz) of B_2P_2 compounds.
(* $[BAr^F{}_4]^-$ signal provided in parentheses, simulated with only chemical shift.)

Compounds	**δ_{iso}* (ppm)**	**Ω (ppm)**	**κ**	**C_Q (MHz)**	**η**	**α (deg.)**	**β (deg.)**	**γ (deg.)**
$[Cu(B_2P_2)]^+[PF_6]^-$	49	94	0.24	4.47	0.13	180	0	90
$[Ag(B_2P_2)]^+[BAr^F{}_4]^-$	52(-6)	108	0.31	4.39	0.04	270	180	90
$[Au(B_2P_2)]^+[BAr^F{}_4]^-$	62 (-7)	133	0.21	4.79	0.03	183	129	41
$[Au(B_2P_2)]^-[K(18\text{-c-}6)]^+$	13	56	0.68	1.43	0.18	60	90	180
B_2P_2 Site 1	60	79	0.53	5.12	0.01	120	4	270
B_2P_2 Site 2	9	34	-0.18	2.91	0.03	15	175	200

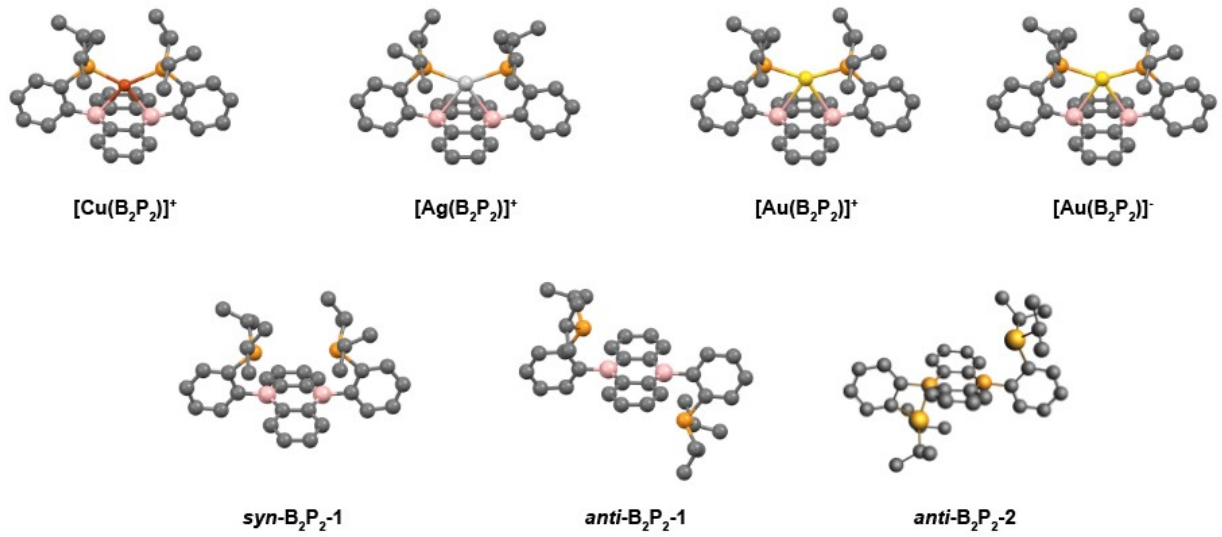


Figure S2. DFT Optimized $M(B_2P_2)^{+/-}$ and B_2P_2 Structures. Hydrogens are omitted for clarity.

Table S4. DFT calculated parameters for B_2P_2.

PBE/M(SDD)	Sum of Angles Around B1(°)	B1-P (Å)	Sum of Angles Around B2 (°)	B2-P (Å)
***syn*-B_2P_2**	358.70	2.80	358.68	2.80
***anti*-B_2P_2 - 1**	359.80	3.08	359.80	3.01
***anti*-B_2P_2 – 2**	353.99	2.25	359.98	3.06

Table S5. Experimental distances for $M[B_2P_2]^{+/-}$ from X-ray diffraction studies in Angstroms (Å).

Crystal Structure	M-B1	M-B2	M-B avg	M-P1	M-P2	M-P avg	M-B-P	M-B-P	M-B-P avg
$[Cu(B_2P_2)]^+$ $[PF_6]^-$	2.33	2.36	**2.35**	2.28	2.29	2.29	78.18	78.64	78.41
$[Cu(B_2P_2)]^+$ $[BAr^F{}_4]^-$	2.34	2.40	**2.37**	2.30	2.29	2.29	77.47	78.54	78.01
$[Ag(B_2P_2)]^+$ $[BAr^F{}_4]^-$	2.54	2.59	**2.57**	2.42	2.41	2.41	75.33	76.37	75.85
$[Au(B_2P_2)]^+$ $[BAr^F{}_4]^-$	2.68	2.61	**2.64**	2.34	2.33	2.33	74.63	75.90	75.27
$[Au(B_2P_2)]^-$ $[K(18\text{-}c\text{-}6)]^+$	2.24	2.24	**2.24**	2.38	2.37	2.38	84.54	84.99	84.77

Table S6. Experimental sum of angles in $M[B_2P_2]^{+/-}$ compounds (°).

Crystal Structure	Sum of Angles Around M	Sum of Angles Around B1	Sum of Angles Around B2
$[Cu(B_2P_2)]^+$ $[PF_6]^-$	358.33	359.92	359.97
$[Cu(B_2P_2)]^+$ $[BAr^F{}_4]^-$	360.01	359.99	359.99
$[Ag(B_2P_2)]^+$ $[BAr^F{}_4]^-$	360.03	360.00	359.98
$[Au(B_2P_2)]^+$ $[BAr^F{}_4]^-$	360.01	359.88	359.95
$[Au(B_2P_2)]^-$ $[K(18\text{-}c\text{-}6)]^+$	359.88	343.84	343.9

Table S7. DFT calculated parameters for $M[B_2P_2]^{+/-}$ compounds in Angstroms (Å).

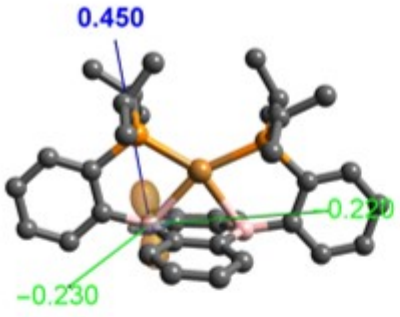
PBE/M(SDD)	M-B1	M-B2	M-B avg	M-P1	M-P2	M-P avg	M-B-P	M-B-P	M-B-P avg
$[Cu(B_2P_2)]^+$	2.37	2.36	**2.37**	2.33	2.33	2.33	78.14	78.18	78.16
$[Ag(B_2P_2)]^+$	2.56	2.56	**2.56**	2.45	2.45	2.45	76.18	76.16	76.17
$[Au(B_2P_2)]^+$	2.71	2.71	**2.71**	2.39	2.39	2.39	74.83	74.83	74.83
$[Au(B_2P_2)]^-$	2.27	2.27	**2.27**	2.48	2.48	2.48	84.24	84.25	84.25

Table S8. DFT calculated parameters for the sum of angles in $M[B_2P_2]^{+/-}$ compounds (°).

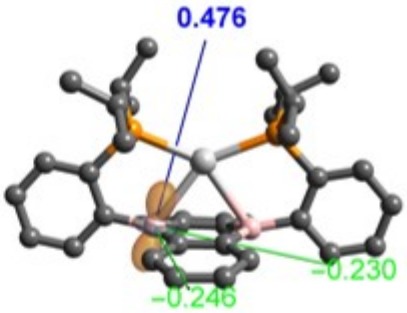
PBE/M(SDD)	Sum of Angles Around M	Sum of Angles Around B1	Sum of Angles Around B2
$[Cu(B_2P_2)]^+$	360.00	359.96	359.96
$[Ag(B_2P_2)]^+$	360.01	359.82	359.82
$[Au(B_2P_2)]^+$	360.01	359.61	359.61
$[Au(B_2P_2)]^-$	360.70	343.43	343.41

Table S9. Calculated ^{11}B NMR parameters of B_2P_2 compounds with ADF (PBE, tDZ / B(QZ4P).

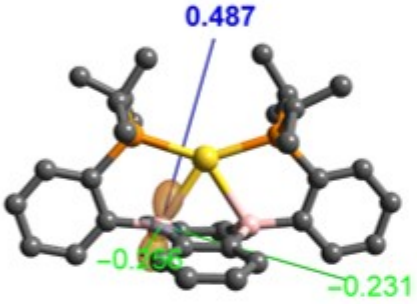
Compounds	δ_{iso} (ppm)	Ω (ppm)	κ	C_Q (MHz)	η	α (deg.)	β (deg.)	γ (deg.)
$[Cu(B_2P_2)]^+$	41	109	0.07	4.29	0.02	118	4	85
$[Ag(B_2P_2)]^+$	47	116	0.10	4.54	0.03	255	151	90
$[Au(B_2P_2)]^+$	49	119	0.11	4.64	0.05	278	148	89
$[Au(B_2P_2)]^-$	5	56	0.22	1.75	0.18	88	99	102
***syn*-B_2P_2**	47	96	0.20	4.65	0.07	90	163	270
***anti*-B_2P_2 – 1**	56	105	0.20	4.85	0.06	80	4	275
***anti*-B_2P_2 – 2; B1**	9	38	0.22	3.26	0.13	85	12	272
***anti*-B_2P_2 – 2; B2**	55	102	0.24	4.77	0.07	90	163	281



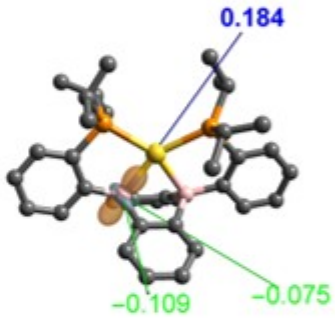
$(B_2P_2)Cu^+$



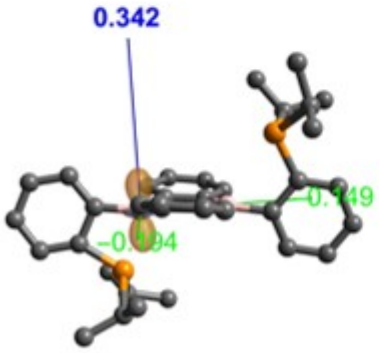
$(B_2P_2)Ag^+$



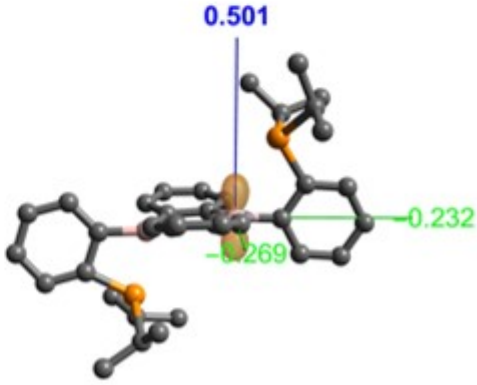
$(B_2P_2)Au^+$



$(B_2P_2)Au^-$



anti-B_2P_2 – 2 (B1)



anti-B_2P_2 – 2 (B2)

Figure S3. Calculated electric field gradient tensors of B_2P_2 plotted with TensorView 1.4.[1]

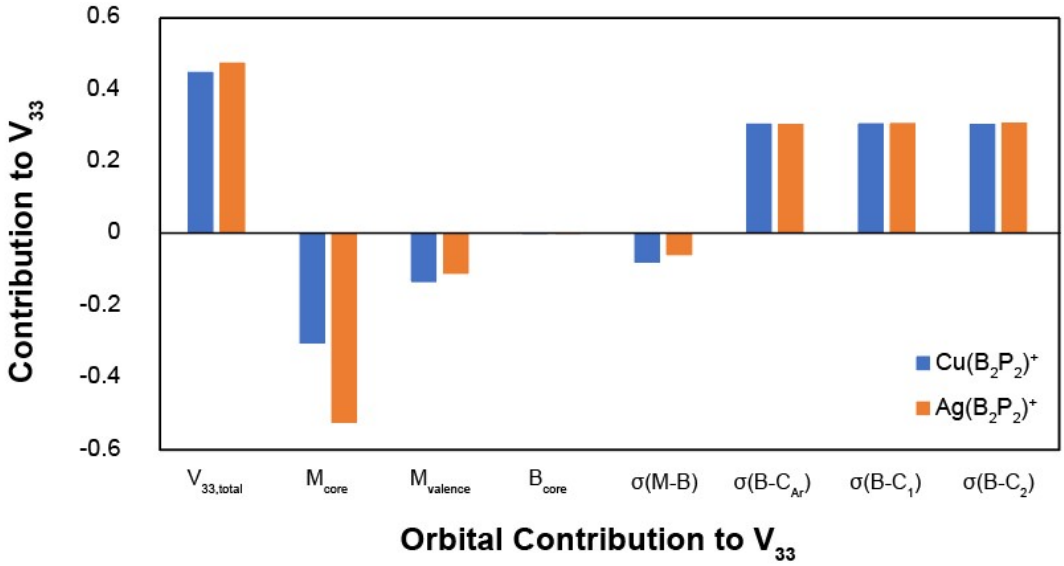


Figure S4. Orbital contributions to V_{33} for $M(B_2P_2)^+$ for M = Cu, Ag.

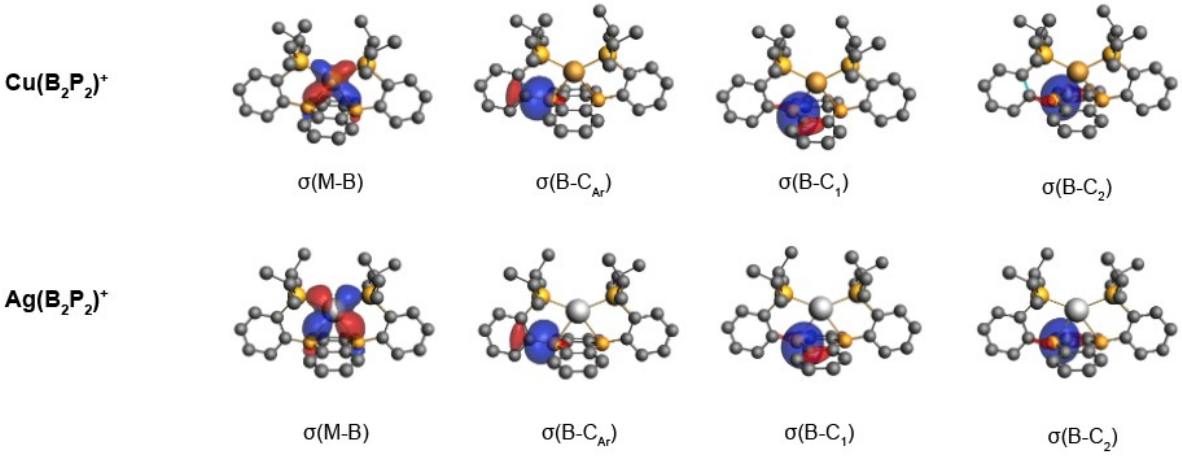


Figure S5. NLMO plots of relevant orbitals in $M(B_2P_2)^+$ for M = Cu, Ag.

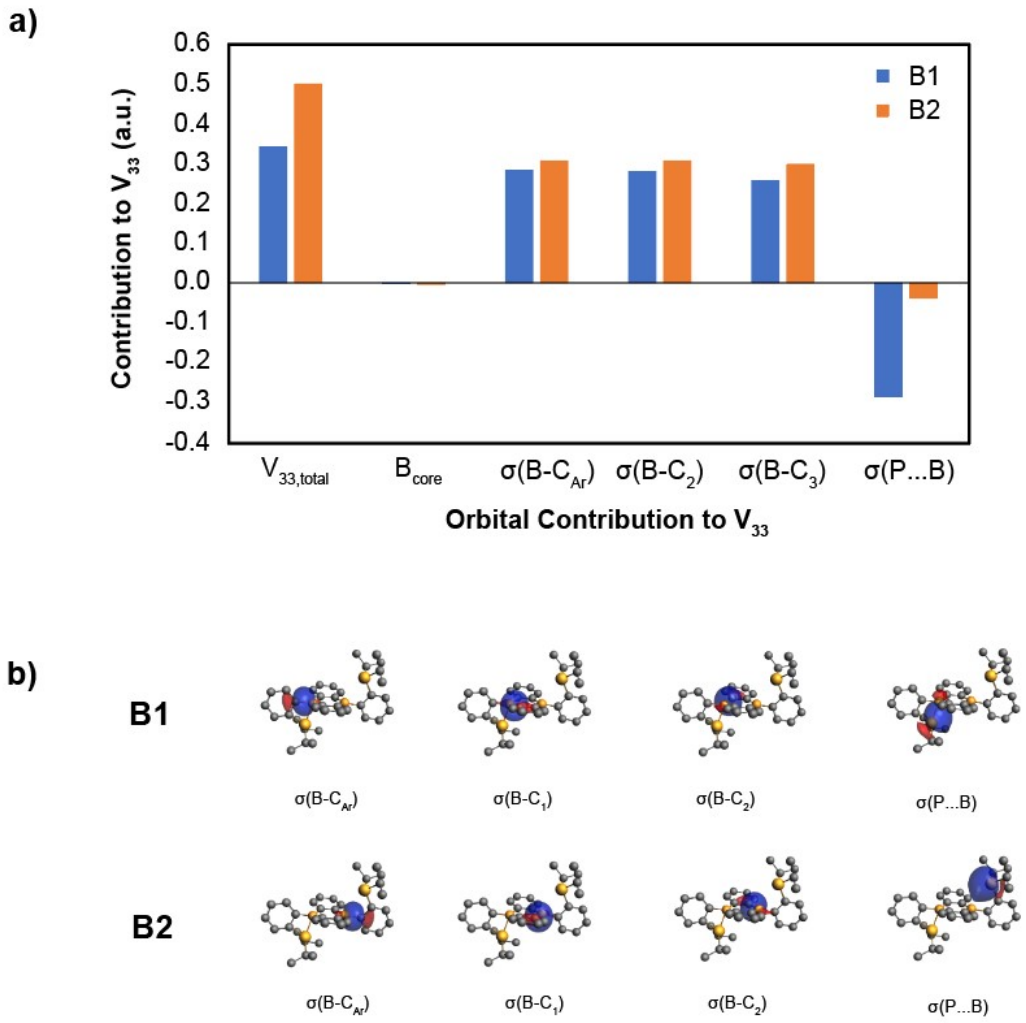
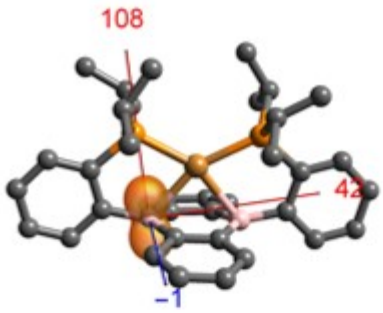


Figure S6. Orbital contributions to V_{33} (a) and NLMO plots of relevant orbitals (b) in B_2P_2.

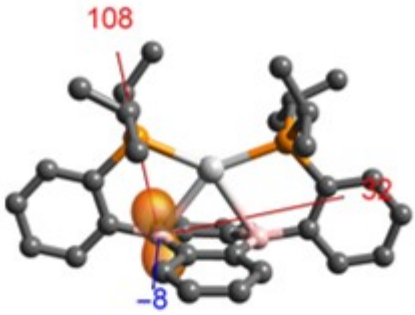
Table S10. NLMO Contributions from major contributors to V_{33} for boron.

Contributions	$[(B_2P_2)Cu]^+$	$[(B_2P_2)Ag]^+$	$[(B_2P_2)Au]^+$	$[(B_2P_2)Au]^-$
V_{33}, total	0.461	0.483	0.488	0.188
Sum of M core:	-0.307	-0.529	-0.850	-1.483
Sum of B core:	-0.001	-0.001	0.001	0.007
Sum of other core:	0.127	0.199	0.295	0.533
Sum of M valence:	-0.136	-0.113	-0.095	-0.155
Sum of other valence:	-0.056	0.069	0.260	0.914
σ(M…B)	-0.081	-0.061	-0.051	-0.127
σ(B-C_{Ar})	0.304	0.304	0.306	0.264
σ(B-C_1)	0.306	0.308	0.311	0.265
σ(B-C_2)	0.305	0.307	0.311	0.227
σ(B…M…B)	*N/A*	*N/A*	*N/A*	-0.257

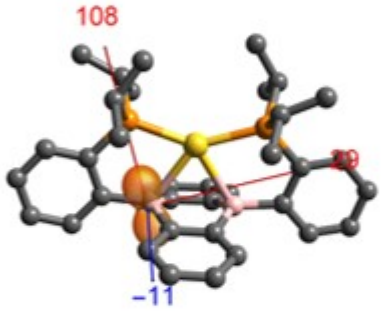
Contribution	B_2P_2 – B1	B_2P_2 – B2
V_{33}, total	0.343	0.509
Sum of B core:	-0.002	-0.005
Sum of other core:	-0.096	-0.013
Sum of other valence:	-0.092	-0.387
σ(P…B)	-0.287	-0.039
σ(B-C_{Ar})	0.257	0.299
σ(B-C_1)	0.280	0.307
σ(B-C_2)	0.283	0.307



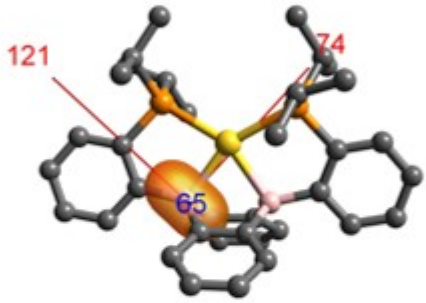
$(B_2P_2)Cu^+$



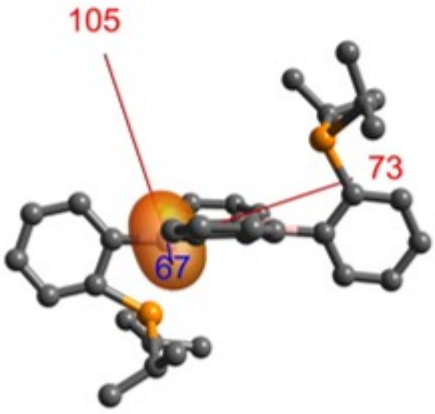
$(B_2P_2)Ag^+$



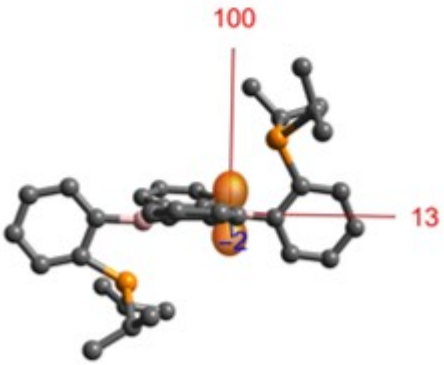
$(B_2P_2)Au^+$



$(B_2P_2)Au^-$



anti-B_2P_2 – 2 (B1)



anti-B_2P_2 – 2 (B2)

Figure S7. Calculated chemical shielding tensors plotted with TensorView 1.4.[1]

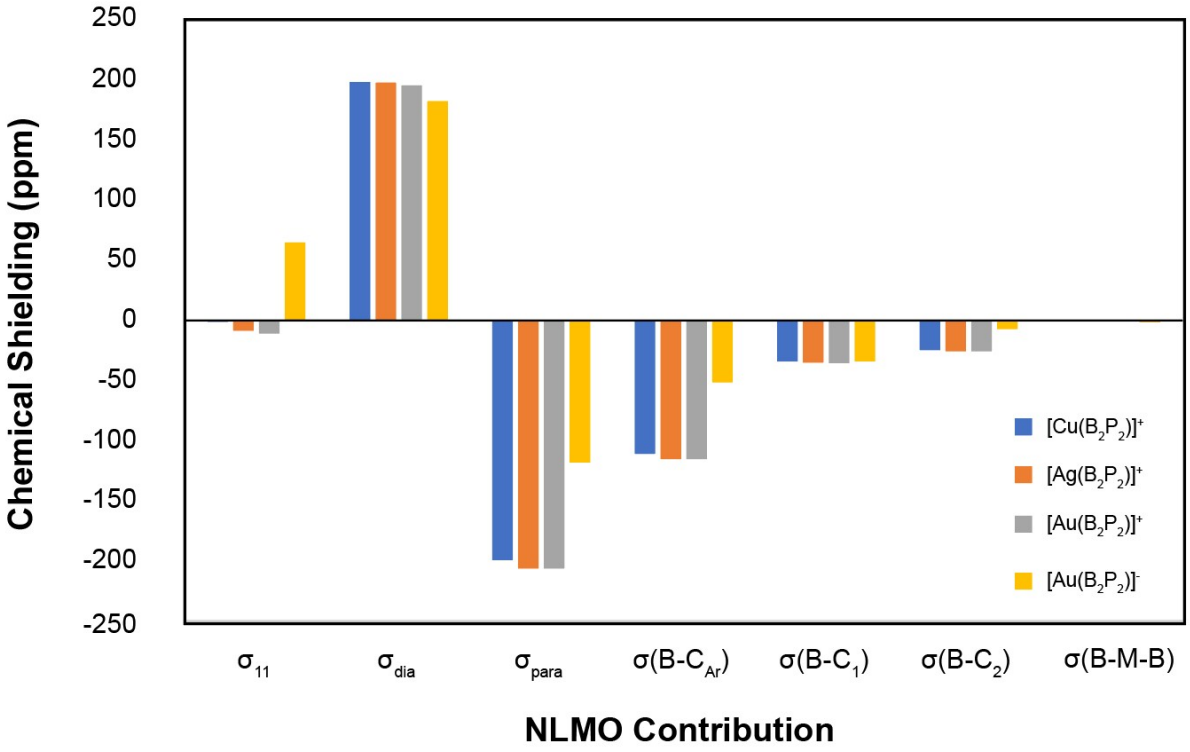


Figure S8. Orbital contributions to σ_{11} for $M(B_2P_2)^{+/-}$ for M = Cu, Ag, Au.

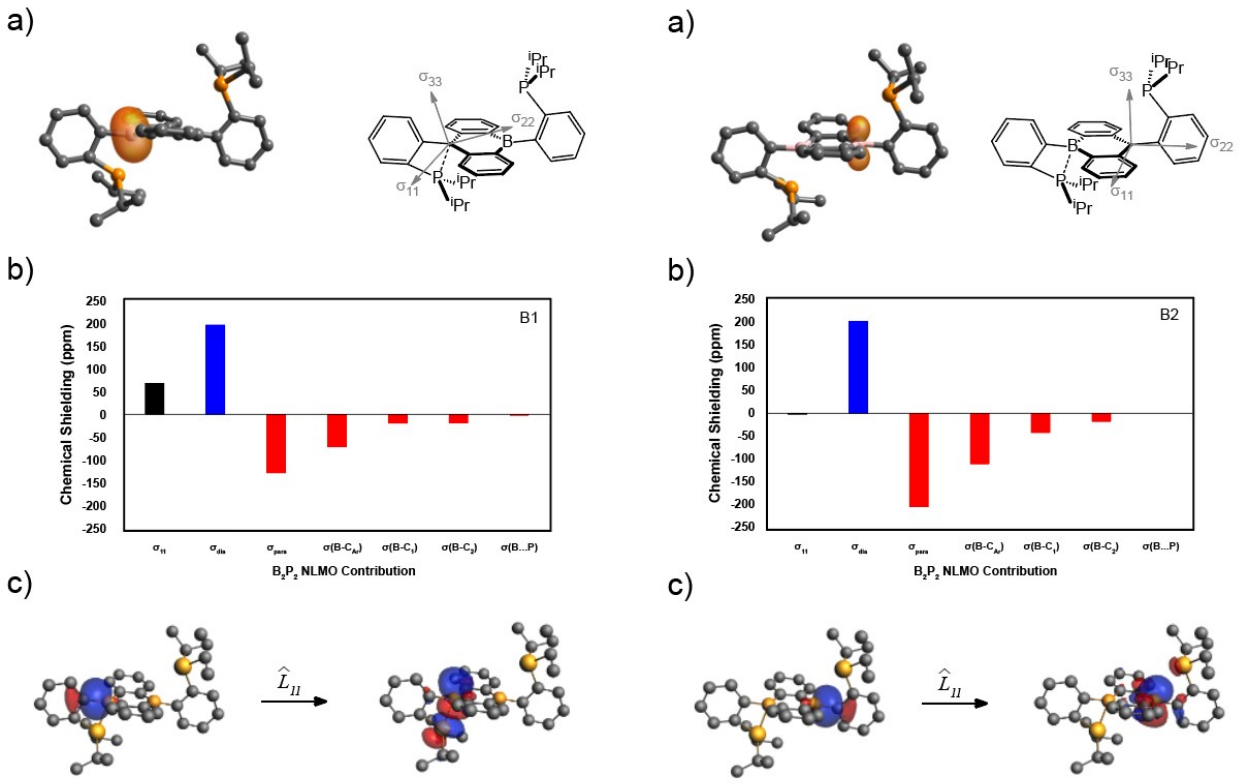


Figure S9. Chemical shielding tensor (CST) plot and schematic with axes (a), NLMO contributions to σ_{11} (b), and major NLMO contributor to σ_{11} deshielding for ***anti*-B_2P_2 - 2**. σ_{11} is pointing towards the reader. Hydrogens are omitted for clarity, and the CST on the schematic is shown with the boron hidden for clarity of axes.

Table S11. NLMO Contributions from boron interactions to σ_{11}, the most deshielded component.

Contribution	$Cu(B_2P_2)^+$			$Ag(B_2P_2)^+$		
	B1	**B2**	**average**	**B1**	**B2**	**average**
σ_{11}, total	-1	-1	-1	-8	-8	-8
σ_{11}, dia.	198	198	198	198	198	198
σ_{11}, para.	-199	-199	-199	-206	-206	-206
σ(B-C_{Ar})	-111	-111	-111	-115	-115	-115
σ(B-C_1)	-33	-34	-34	-35	-35	-35
σ(B-C_2)	-25	-24	-24	-25	-25	-25

Contribution	$Au(B_2P_2)^+$			$Au(B_2P_2)^-$		
	B1	**B2**	**average**	**B1**	**B2**	**average**
σ_{11}, total	-11	-11	-11	65	65	65
σ_{11}, dia.	195	195	195	182	182	182
σ_{11}, para.	-206	-206	-206	-118	-118	-118
σ(B-C_{Ar})	-115	-115	-115	-51	-51	-51
σ(B-C_1)	-35	-35	-35	-34	-34	-34
σ(B-C_2)	-26	-26	-26	-7	-7	-7
σ(B…Au…B)	--	--	--	-1	-1	-1

Contribution	*syn*-B_2P_2	*anti*-B_2P_2 - 1	*anti*-B_2P_2 - 2	
	B_{avg}	B_{avg}	**B1**	**B2**
σ_{11}, total	-4	-4	-2	67
σ_{11}, dia.	200	198	200	194
σ_{11}, para.	-204	-192	-202	-127
σ(B-C_{Ar})	-112	-105	-110	-70
σ(B-C_1)	-41	-46	-42	-19
σ(B-C_2)	-19	-17	-18	-19
σ(P…B)	--	--	--	-2

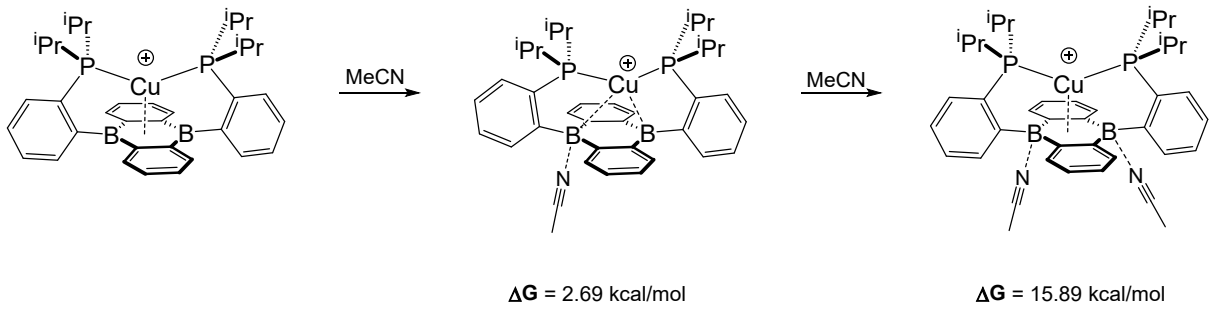


Figure S10. Gibbs Energies for MeCN binding to $Cu(B_2P_2)^+$.

Table 12. Calculated ^{11}B NMR Parameters and Delocalization Energies for $Cu(B_2P_2)^+$ * n(MeCN) for n = 1,2

Compounds		δ_{iso} (ppm)	Ω (ppm)	C_Q (MHz)	Delocalization Energy d_{Cu} --> p_B / σ(B…NCMe) (kcal/mol)
$[Cu(B_2P_2)]^+$ * (MeCN)	Cu…**B**R_3	37	96	3.91	4.71
	Cu…**B**R_3(NCMe)	-13	26	2.55	0.16
$[Cu(B_2P_2)]^+$ * 2(MeCN)	Cu…**B**R_3(NCMe)	-13	23	2.58	0.15
	Cu…**B**R_3(NCMe)	-13	23	2.58	0.17

$[(B_2P_2)Cu]^+$

Cu	0.00033300	0.09156600	0.00433100
B	1.49276500	-1.74237400	-0.01478300
C	0.74495600	-1.93453200	1.34500900
C	1.44891000	-2.11257300	2.56483600
H	2.54379900	-2.12756400	2.54975900
C	0.76768200	-2.30168100	3.76842100
H	1.32444600	-2.48296700	4.69301700
C	-0.64197000	-2.25650100	3.79646200
H	-1.17166200	-2.40275000	4.74294700
C	-1.35964900	-2.03231400	2.62004900
H	-2.45360000	-1.99656300	2.64971900
C	-0.69639600	-1.90149900	1.37087600
B	-1.49425500	-1.74179400	0.03015200
C	-0.74648900	-1.95034200	-1.32724900
C	-1.45038200	-2.14219000	-2.54485700
H	-2.54529700	-2.15628700	-2.52996600
C	-0.76909400	-2.34523600	-3.74627300
H	-1.32590600	-2.53686800	-4.66875400
C	0.64045300	-2.30046300	-3.77480300
H	1.17019900	-2.45731400	-4.71955500
C	1.35806500	-2.06271500	-2.60089200
H	2.45201600	-2.02687100	-2.63103500
C	0.69476600	-1.91781900	-1.35344300
P	2.07032300	1.16084200	-0.02693900
C	3.04035000	-1.42816700	-0.05716000
C	3.43894100	-0.06787400	-0.10698700
C	4.79963200	0.28344100	-0.23034500
H	5.10618400	1.33059100	-0.30442900
C	5.77756800	-0.71904900	-0.27262400
H	6.83251000	-0.44630600	-0.36641200
C	5.40008200	-2.06829700	-0.19851500
H	6.16384200	-2.85105400	-0.23031400
C	4.04566100	-2.41805900	-0.09919200
H	3.76606100	-3.47643100	-0.06365100
C	2.41053400	2.32287100	-1.46759600
H	3.48057600	2.58380800	-1.36293300
C	2.22297100	1.58860300	-2.80375400
H	1.17018200	1.30038900	-2.95924900
H	2.83790400	0.67749000	-2.86370400
H	2.51590300	2.25113300	-3.63508800
C	1.58522700	3.61536300	-1.39977100
H	1.83051400	4.25374400	-2.26473900
H	1.78261500	4.20289700	-0.48956300
H	0.50398700	3.40436800	-1.44372600
C	2.33111500	2.20397000	1.52446400
H	1.51577800	2.94900800	1.45945000
C	3.67209500	2.95203100	1.58364400
H	3.67457900	3.61788800	2.46302000
H	3.85960400	3.57907300	0.69764900
H	4.51348700	2.25145600	1.70137800
C	2.11615400	1.35315500	2.78457000
H	2.88919500	0.57234400	2.87043800
H	1.13392900	0.85461800	2.79231000
H	2.18363800	1.99196200	3.68088000
P	-2.06982500	1.16143700	0.01564500
C	-3.04164100	-1.42646700	0.06952600
C	-3.43928100	-0.06551000	0.10750100
C	-4.79967900	0.28780600	0.22808200
H	-5.10552900	1.33575900	0.29300200
C	-5.77826900	-0.71361700	0.27954700
H	-6.83298900	-0.43931500	0.37128600
C	-5.40175200	-2.06372100	0.21715400
H	-6.16604400	-2.84563300	0.25612500
C	-4.04759700	-2.41527100	0.12041400
H	-3.76870800	-3.47410000	0.09414700
C	-2.32872400	2.18823000	-1.54691800
H	-1.51233600	2.93273800	-1.48957800

C	-2.11477800	1.32406000	-2.79803300
H	-2.88896000	0.54352800	-2.87602700
H	-1.13326900	0.82417400	-2.80011600
H	-2.18105600	1.95357800	-3.70096800
C	-3.66874800	2.93730900	-1.61379000
H	-3.67033200	3.59431500	-2.49980400
H	-3.85551300	3.57329900	-0.73406100
H	-4.51103700	2.23667300	-1.72455100
C	-2.40981900	2.33915700	1.44354600
H	-3.47949500	2.60048800	1.33603500
C	-2.22302400	1.61892700	2.78739400
H	-1.17060100	1.33086200	2.94570200
H	-2.83913700	0.70929800	2.85708300
H	-2.51484000	2.29064500	3.61171100
C	-1.58244200	3.62947100	1.36179500
H	-1.82632500	4.27755600	2.21992400
H	-1.77896600	4.20767700	0.44546000
H	-0.50156700	3.41691600	1.40762900

$[(B_2P_2)Ag]^+$

Ag	-0.00012700	0.31352900	0.00016900
B	-1.49504100	-1.76888500	-0.03244200
C	-0.68914900	-1.97350200	-1.36755200
C	-1.34182500	-2.13875400	-2.61415500
H	-2.43579100	-2.10511700	-2.65332000
C	-0.61473900	-2.38020000	-3.78488400
H	-1.13852700	-2.54621600	-4.73135400
C	0.79209000	-2.41177600	-3.74772600
H	1.35747200	-2.60293500	-4.66505600
C	1.46480400	-2.19404800	-2.54074700
H	2.55984900	-2.19665600	-2.52121100
C	0.75425800	-1.99522600	-1.33191900
B	1.49530800	-1.76878300	0.03270600
C	0.68941600	-1.97321300	1.36783900
C	1.34210900	-2.13820900	2.61447100
H	2.43607300	-2.10449100	2.65361500
C	0.61504900	-2.37951900	3.78524100
H	1.13885300	-2.54531100	4.73174100
C	-0.79178000	-2.41123400	3.74809300
H	-1.35714200	-2.60230400	4.66545400
C	-1.46451900	-2.19378000	2.54108000
H	-2.55956300	-2.19651800	2.52153500
C	-0.75399100	-1.99508800	1.33221700
C	-3.04776200	-1.45412000	-0.08117700
C	-3.52821500	-0.11748600	-0.11442200
C	-4.90838000	0.15244800	-0.23571000
H	-5.27181100	1.18281300	-0.29090900
C	-5.82887200	-0.90128100	-0.29791300
H	-6.89732000	-0.68766600	-0.39152300
C	-5.37322900	-2.22639100	-0.24258300
H	-6.08835200	-3.05309000	-0.28933100
C	-4.00097300	-2.49637900	-0.14137100
H	-3.66293200	-3.53811900	-0.11876300
P	-2.27496400	1.22591600	-0.02090600
C	-2.63943400	2.36321700	-1.46819800
H	-3.71265500	2.62041000	-1.38879700
C	-2.40931500	1.61172600	-2.78867700
H	-2.68163000	2.25912400	-3.63873500
H	-3.01354200	0.69355600	-2.85224200
H	-1.34863300	1.33001000	-2.90558400
C	-1.80967900	3.65380100	-1.39319000
H	-0.72816000	3.43144800	-1.40244500
H	-2.02998500	4.25180800	-0.49481200
H	-2.02619400	4.28409100	-2.27166200
C	-2.58514800	2.23065800	1.54202500
H	-1.79822300	3.00770400	1.48811600
C	-2.32457300	1.36104300	2.78187000
H	-2.40586600	1.97637700	3.69331700
H	-1.32214500	0.90152100	2.76668800
H	-3.06519200	0.54814100	2.85800100
C	-3.95676600	2.91853100	1.61149300
H	-4.76765300	2.17973800	1.70961400
H	-4.16479300	3.55275300	0.73484100
H	-3.99463400	3.56708400	2.50288200
C	3.04800900	-1.45394800	0.08133600
C	3.52831900	-0.11725800	0.11429700
C	4.90847100	0.15284800	0.23533200
H	5.27180200	1.18325700	0.29030200
C	5.82907500	-0.90077700	0.29758700
H	6.89751700	-0.68703600	0.39097700
C	5.37356400	-2.22595000	0.24258400
H	6.08878700	-3.05255600	0.28941200
C	4.00132500	-2.49610700	0.14160800
H	3.66338600	-3.53788400	0.11923200
P	2.27484600	1.22591400	0.02077700
C	2.63938000	2.36344800	1.46786000
H	3.71259300	2.62065600	1.38833600

C	2.40936500	1.61218700	2.78848800
H	2.68173900	2.25973300	3.63841600
H	3.01360200	0.69403300	2.85217800
H	1.34869200	1.33048700	2.90551200
C	1.80959600	3.65401600	1.39275400
H	0.72807800	3.43165200	1.40209300
H	2.02982200	4.25194400	0.49430400
H	2.02614700	4.28439500	2.27115000
C	2.58469000	2.23051600	-1.54231300
H	1.79771400	3.00750500	-1.48836200
C	2.32395600	1.36073500	-2.78200900
H	2.40503900	1.97595700	-3.69355000
H	1.32156500	0.90114100	-2.76657700
H	3.06462800	0.54788000	-2.85816400
C	3.95625400	2.91846000	-1.61214000
H	4.76715000	2.17969600	-1.71038900
H	4.16445900	3.55274800	-0.73558100
H	3.99388600	3.56694100	-2.50359000

$[(B_2P_2)Au]^+$

Au	0.00009000	0.44369000	0.00001200
B	1.47893100	-1.82538200	-0.03988600
C	0.75891900	-2.08042900	1.33033100
C	1.47692000	-2.30375900	2.52790000
H	2.57202400	-2.30734700	2.50324600
C	0.81030400	-2.54365000	3.73575100
H	1.38077900	-2.75105700	4.64641800
C	-0.59530700	-2.51313400	3.78071000
H	-1.11449200	-2.69591100	4.72666300
C	-1.32869500	-2.25056000	2.61674700
H	-2.42260100	-2.21846000	2.66285400
C	-0.68092200	-2.05992900	1.37369700
B	-1.47930000	-1.82550300	0.03995000
C	-0.75929500	-2.08061000	-1.33024400
C	-1.47729100	-2.30408300	-2.52778800
H	-2.57239500	-2.30787700	-2.50309600
C	-0.81067200	-2.54386500	-3.73565900
H	-1.38114200	-2.75131900	-4.64631900
C	0.59493300	-2.51315100	-3.78064500
H	1.11412700	-2.69584400	-4.72661000
C	1.32831200	-2.25049900	-2.61669600
H	2.42221400	-2.21830300	-2.66282700
C	0.68054600	-2.05993600	-1.37362700
C	3.02928800	-1.50401800	-0.09619700
C	3.51223200	-0.17017100	-0.12392600
C	4.89177400	0.10251100	-0.25132200
H	5.25576000	1.13289100	-0.30213000
C	5.81084500	-0.95109400	-0.32539600
H	6.87878800	-0.73751300	-0.42391300
C	5.35391600	-2.27620100	-0.27604500
H	6.06817000	-3.10307400	-0.33217400
C	3.98232600	-2.54605100	-0.16895400
H	3.64354800	-3.58753300	-0.15130300
P	2.27444700	1.17964700	-0.01375700
C	2.58161400	2.16804100	1.55629200
H	1.79860300	2.94893100	1.50685900
C	2.31792200	1.28852800	2.78825500
H	3.05556600	0.47250200	2.85843500
H	1.31372800	0.83426600	2.76469800
H	2.40112000	1.89704500	3.70396700
C	3.95789200	2.84721200	1.62546600
H	3.99958800	3.48930300	2.52111100
H	4.16768000	3.48664700	0.75299700
H	4.76502200	2.10374600	1.71812300
C	2.62207300	2.31946900	-1.45948400
H	3.69889400	2.56374500	-1.38674400
C	2.37250600	1.57584900	-2.78096800
H	1.30795000	1.30653200	-2.88692500
H	2.96611200	0.65155700	-2.85462500
H	2.64476300	2.22521300	-3.62933800
C	1.80628600	3.61779400	-1.36892700
H	2.01925000	4.24837300	-2.24790500
H	2.04348100	4.21037900	-0.47124300
H	0.72361800	3.40305000	-1.36456800
C	-3.02959600	-1.50387500	0.09621800
C	-3.51225500	-0.16992000	0.12384500
C	-4.89175300	0.10305500	0.25112500
H	-5.25552100	1.13351300	0.30184900
C	-5.81105400	-0.95034700	0.32519800
H	-6.87895900	-0.73653700	0.42361800
C	-5.35440100	-2.27555400	0.27598200
H	-6.06883300	-3.10227300	0.33212300
C	-3.98286200	-2.54569800	0.16899100
H	-3.64430700	-3.58725300	0.15143500
P	-2.27424800	1.17969800	0.01370800
C	-2.58121400	2.16819400	-1.55628600
H	-1.79809300	2.94898000	-1.50678200

C	-2.31756800	1.28868200	-2.78826800
H	-3.05518300	0.47262000	-2.85838200
H	-1.31336100	0.83444000	-2.76476500
H	-2.40085200	1.89717800	-3.70398600
C	-3.95736700	2.84761000	-1.62556900
H	-3.99885800	3.48972200	-2.52120800
H	-4.16709400	3.48707900	-0.75310400
H	-4.76463700	2.10430400	-1.71828700
C	-2.62180300	2.31954500	1.45947600
H	-3.69859200	2.56393400	1.38667900
C	-2.37238600	1.57588700	2.78095900
H	-1.30785800	1.30647100	2.88697600
H	-2.96609400	0.65166200	2.85460300
H	-2.64461900	2.22528400	3.62931500
C	-1.80590400	3.61780100	1.36900800
H	-2.01899800	4.24842400	2.24792700
H	-2.04290100	4.21038000	0.47126600
H	-0.72324900	3.40299700	1.36486600

$[(B_2P_2)Au]^-$

Au	-0.00007800	-0.29450500	-0.00036700
B	1.29909600	1.55397500	0.16409500
C	0.87069600	2.31119600	-1.21424500
C	1.68915800	2.91114200	-2.18141600
H	2.77967800	2.92139600	-2.04504100
C	1.13360900	3.48341100	-3.35001300
H	1.78850900	3.93434800	-4.10656600
C	-0.25005500	3.45682700	-3.54461500
H	-0.68674400	3.88389000	-4.45647500
C	-1.08712100	2.86798200	-2.56761400
H	-2.17177300	2.84148100	-2.73989200
C	-0.54874800	2.29636400	-1.40607400
B	-1.29922600	1.55426500	-0.16393300
C	-0.87085000	2.30942100	1.21562900
C	-1.68933000	2.90785000	2.18371900
H	-2.77984800	2.91836000	2.04731800
C	-1.13377900	3.47820900	3.35325400
H	-1.78867200	3.92797400	4.11051000
C	0.24988200	3.45124100	3.54784300
H	0.68656400	3.87684900	4.46039000
C	1.08696200	2.86393500	2.56992500
H	2.17161700	2.83714700	2.74215600
C	0.54859200	2.29424100	1.40743800
C	2.85312900	1.16965600	0.34208800
C	3.37654500	-0.15346500	0.28723200
C	4.75382100	-0.40762300	0.48121800
H	5.13797700	-1.43370100	0.45248600
C	5.64863300	0.64294000	0.71845600
H	6.71345500	0.43576900	0.87192200
C	5.16245500	1.95967900	0.75455200
H	5.85233600	2.79320500	0.93264900
C	3.79627400	2.20673100	0.57080600
H	3.42951000	3.23882100	0.60980000
P	2.16757200	-1.50653200	-0.06494000
C	2.53772200	-2.04698400	-1.84688300
H	1.86149100	-2.91099800	-1.99619100
C	2.10938800	-0.92986300	-2.81258200
H	2.71429400	-0.02019200	-2.66592900
H	1.05875300	-0.63581600	-2.65533100
H	2.23567400	-1.26200800	-3.85917800
C	3.98017900	-2.49627300	-2.11508200
H	4.08487800	-2.82776100	-3.16457000
H	4.29167200	-3.33584300	-1.47028400
H	4.68512800	-1.66354900	-1.95675900
C	2.80104400	-2.95736300	0.98246100
H	3.86961800	-3.12658600	0.74719400
C	2.67683300	-2.59032900	2.46955900
H	1.62575700	-2.38268200	2.73485900
H	3.26601800	-1.69309400	2.71582800
H	3.03054700	-3.42290800	3.10443600
C	2.01793600	-4.23727000	0.65771500
H	2.33091200	-5.06206800	1.32334000
H	2.17257300	-4.57081200	-0.38202100
H	0.93477000	-4.07738300	0.80262900
C	-2.85321500	1.16979600	-0.34193300
C	-3.37651900	-0.15338400	-0.28723900
C	-4.75382900	-0.40760700	-0.48093400
H	-5.13787500	-1.43373000	-0.45241900
C	-5.64880500	0.64292000	-0.71768000
H	-6.71364500	0.43569400	-0.87093100
C	-5.16274800	1.95971100	-0.75354800
H	-5.85274400	2.79323100	-0.93123300
C	-3.79654200	2.20683400	-0.57011800
H	-3.42992100	3.23898200	-0.60885800
P	-2.16746500	-1.50657800	0.06433900
C	-2.53778200	-2.04834700	1.84582000
H	-1.86128000	-2.91224100	1.99460500

C	-2.10975500	-0.93162000	2.81212200
H	-2.71498000	-0.02208300	2.66600400
H	-1.05924400	-0.63707400	2.65492500
H	-2.23581400	-1.26434800	3.85856000
C	-3.98007500	-2.49829100	2.11370500
H	-4.08457200	-2.83087600	3.16286400
H	-4.29136000	-3.33729700	1.46806600
H	-4.68528100	-1.66562700	1.95626600
C	-2.80038700	-2.95658700	-0.98441900
H	-3.86905800	-3.12603900	-0.74969600
C	-2.01737100	-4.23675500	-0.66052100
H	-0.93420700	-4.07678800	-0.80527300
H	-2.33036900	-5.06104300	-1.32676100
H	-2.17205000	-4.57104400	0.37896800
C	-2.67570400	-2.58836500	-2.47119700
H	-1.62452100	-2.38065500	-2.73601800
H	-3.26471700	-1.69086900	-2.71692400
H	-3.02932400	-3.42041100	-3.10682700

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B	1.50023400	-1.50636600	0.03903900
C	0.68398800	-1.72299500	1.36389500
C	1.33449200	-1.97393700	2.59250700
H	2.43002300	-1.97290300	2.62364600
C	0.61256800	-2.23784800	3.76527700
H	1.14013100	-2.44428400	4.70245500
C	-0.78983200	-2.23794900	3.73103200
H	-1.36185400	-2.44468700	4.64178200
C	-1.45614000	-1.97581700	2.52509400
H	-2.55171400	-1.97878700	2.50526500
C	-0.74853400	-1.72307500	1.32927900
B	-1.49864400	-1.50714000	-0.03789700
C	-0.68234600	-1.72432800	-1.36259300
C	-1.33279700	-1.97637100	-2.59101700
H	-2.42832900	-1.97569000	-2.62213200
C	-0.61081300	-2.24095600	-3.76359400
H	-1.13831600	-2.44823000	-4.70062000
C	0.79158600	-2.24067300	-3.72933000
H	1.36366800	-2.44799300	-4.63991100
C	1.45783800	-1.97739400	-2.52360500
H	2.55341500	-1.98000800	-2.50380600
C	0.75018000	-1.72389600	-1.32799300
P	2.28603600	1.17487200	-0.08309600
C	3.08948000	-1.38756300	0.06646900
C	3.63538500	-0.08143900	-0.02977800
C	5.02830700	0.11897100	-0.09453500
H	5.44044200	1.12764400	-0.19971200
C	5.89413800	-0.98215500	-0.03570500
H	6.97707500	-0.83095900	-0.08541500
C	5.36907800	-2.27840100	0.08696200
H	6.04661200	-3.13717100	0.13547100
C	3.98172700	-2.47991600	0.13452300
H	3.58882200	-3.49972700	0.21278500
C	2.76890300	2.29608300	-1.53096100
H	3.79928200	2.66059200	-1.35381800
C	2.75424400	1.48768000	-2.83742700
H	1.75060300	1.08002500	-3.04356800
H	3.45674100	0.64042700	-2.80047000
H	3.04101400	2.13268900	-3.68651900
C	1.82385400	3.50477700	-1.61738900
H	2.07728700	4.12455100	-2.49514100
H	1.88039800	4.15276900	-0.72765200
H	0.77582800	3.17691100	-1.73307200
C	2.54047400	2.29141200	1.43088400
H	1.75174700	3.05804200	1.29811600
C	3.89853800	2.99811100	1.53850800
H	3.90356300	3.67707000	2.41001500
H	4.13711600	3.60343000	0.64867300
H	4.71069300	2.26779500	1.68686500
C	2.21874900	1.50309300	2.70987400
H	2.95370500	0.69698700	2.87091600
H	1.22159800	1.03799800	2.66685300
H	2.25533900	2.17023700	3.58884300
P	-2.28689400	1.17488900	0.08248100
C	-3.08788800	-1.38886700	-0.06546100
C	-3.63478100	-0.08308500	0.02991200
C	-5.02788800	0.11621000	0.09450100
H	-5.44080800	1.12463100	0.19896600
C	-5.89288900	-0.98559900	0.03639100
H	-6.97594000	-0.83518700	0.08598400
C	-5.36683000	-2.28151500	-0.08541600
H	-6.04367800	-3.14085800	-0.13335600
C	-3.97932500	-2.48194200	-0.13282400
H	-3.58561700	-3.50149600	-0.21040300
C	-2.54249900	2.28979400	-1.43255700
H	-1.75468400	3.05744800	-1.30032000
C	-2.21965900	1.50071900	-2.71078900

H	-2.95372900	0.69370200	-2.87129600
H	-1.22204000	1.03666100	-2.66715000
H	-2.25673000	2.16704300	-3.59036200
C	-3.90134900	2.99485000	-1.54106300
H	-3.90693300	3.67319800	-2.41304700
H	-4.14088700	3.60052100	-0.65171900
H	-4.71261500	2.26349000	-1.68913900
C	-2.77160600	2.29675900	1.52922800
H	-3.80250900	2.65963400	1.35181700
C	-2.75573200	1.48949900	2.83640000
H	-1.75147800	1.08351300	3.04288600
H	-3.45696700	0.64116500	2.80018000
H	-3.04345500	2.13479300	3.68495500
C	-1.82826400	3.50685800	1.61452300
H	-2.08216600	4.12682100	2.49200700
H	-1.88615700	4.15420000	0.72440300
H	-0.77972100	3.18055200	1.72991000

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B	-1.26875800	0.17090600	-0.68685900
C	-0.59454300	-1.20060900	-0.32905700
C	-1.16774600	-2.42339600	-0.74212000
H	-2.07224200	-2.40351700	-1.35881800
C	-0.61378600	-3.65768700	-0.37467600
H	-1.08072400	-4.59114200	-0.70604900
C	0.53563400	-3.69028700	0.42879100
H	0.96393400	-4.64933100	0.73862400
C	1.14097900	-2.48819800	0.82146900
H	2.04875400	-2.51879400	1.43337000
C	0.61491900	-1.23441600	0.43967000
B	1.34571100	0.10079900	0.82229700
C	0.65019900	1.47134200	0.50277100
C	1.20429800	2.69084400	0.94844000
H	2.10548600	2.66790700	1.57062400
C	0.63422300	3.92666700	0.60736500
H	1.08291500	4.85819400	0.96789300
C	-0.50258300	3.96289800	-0.21186200
H	-0.94018500	4.92307100	-0.50433100
C	-1.08619800	2.76157900	-0.64201800
H	-1.98422700	2.79497400	-1.26803100
C	-0.55020300	1.50599500	-0.28118500
P	-3.90807700	-0.20530100	0.85842800
C	-2.59815700	0.20784700	-1.55575300
C	-3.88573500	-0.00437200	-0.98836000
C	-5.02369200	-0.05298100	-1.82168000
H	-6.01069000	-0.24570800	-1.38977100
C	-4.90856600	0.13197200	-3.20580400
H	-5.79950200	0.09050300	-3.84037800
C	-3.64824200	0.37428800	-3.77087100
H	-3.55028800	0.52525100	-4.85077600
C	-2.51110500	0.41264700	-2.95316900
H	-1.53077900	0.58869100	-3.41058500
C	-5.15496100	-1.61093900	1.11690000
H	-6.09936700	-1.35522600	0.59952900
C	-4.60743100	-2.91165700	0.50960100
H	-3.64083600	-3.18768900	0.96320400
H	-4.45615300	-2.81935000	-0.57758300
H	-5.31465200	-3.74175700	0.68398400
C	-5.44783800	-1.78389600	2.61593500
H	-6.12022900	-2.64482800	2.77653600
H	-5.93491900	-0.89869000	3.05583000
H	-4.51994700	-1.97614800	3.18171500
C	-4.87436300	1.30469100	1.50229600
H	-4.90500800	1.10688800	2.59169800
C	-6.31109700	1.49155300	0.99824900
H	-6.78171200	2.35246900	1.50649200
H	-6.94746600	0.61178700	1.18721200
H	-6.32588500	1.70231700	-0.08375500

C	-4.04543600	2.57876900	1.28312600
H	-3.98735000	2.82675700	0.21026600
H	-3.01507600	2.47313800	1.65684500
H	-4.51442600	3.43557000	1.79808600
P	3.80876200	-0.15012400	-0.88971300
C	2.71267100	0.06593300	1.63317900
C	3.95529200	-0.08582400	0.95827100
C	5.15341200	-0.19378500	1.69485600
H	6.10495800	-0.34497800	1.17568000
C	5.13908800	-0.12311000	3.09438600
H	6.07413200	-0.20748600	3.65715100
C	3.92237400	0.05608500	3.76877100
H	3.90517100	0.11478000	4.86187100
C	2.72565600	0.14741500	3.04481600
H	1.78122500	0.26988400	3.58711500
C	4.77455100	1.36003300	-1.53140500
H	4.70769000	1.22166100	-2.62831300
C	4.01804200	2.64913000	-1.17809600
H	4.05125800	2.83955400	-0.09251800
H	2.95912300	2.60261700	-1.47565100
H	4.48170400	3.51538200	-1.68195000
C	6.25492300	1.46755800	-1.14277600
H	6.71679600	2.33374300	-1.65000100
H	6.83711800	0.57489400	-1.42324600
H	6.36803000	1.62576800	-0.05759100
C	4.95788300	-1.58410800	-1.35823900
H	5.95666700	-1.39603900	-0.91959700
C	4.41552500	-2.90114900	-0.78272900
H	3.40224000	-3.11507400	-1.16116900
H	4.36559800	-2.87458400	0.31727900
H	5.07114400	-3.74142000	-1.07204300
C	5.09735500	-1.66660600	-2.88671800
H	5.71614000	-2.53674500	-3.16771500
H	5.57319000	-0.77027800	-3.31645100
H	4.11130800	-1.78953600	-3.36688200

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B	0.97284500	-0.07100800	-0.61353500
C	0.34627200	-1.35571000	0.02503200
C	1.01944200	-2.60003500	-0.03874200
H	1.94048000	-2.67278900	-0.62742700
C	0.55599500	-3.72426600	0.65451900
H	1.10087700	-4.67248700	0.59921900
C	-0.60419200	-3.61861900	1.43753900
H	-0.96112600	-4.48204100	2.00974600
C	-1.31359400	-2.40949700	1.47503100
H	-2.23243200	-2.34741500	2.06999900
C	-0.87706500	-1.27129000	0.76398600
B	-1.72632700	0.08105300	0.73992500
C	-0.90428600	1.41226900	0.41177100
C	-1.35836400	2.68882400	0.80577600
H	-2.26890000	2.76707200	1.41176900
C	-0.67025900	3.85964000	0.45081200
H	-1.04015500	4.83528700	0.78482100
C	0.48522200	3.77928000	-0.34139700
H	1.01108800	4.68991800	-0.64623800
C	0.96666100	2.52055600	-0.72220800
H	1.87612100	2.45307400	-1.33044000
C	0.31743600	1.32300600	-0.33156200
P	3.68667100	-0.01377600	0.79833300
C	2.24208400	-0.18163700	-1.56525400
C	3.56602000	-0.22169800	-1.04573000
C	4.66153500	-0.38947200	-1.91843900
H	5.67853900	-0.44593000	-1.51607100
C	4.46719900	-0.49752400	-3.30185500
H	5.32591300	-0.63078100	-3.96763700

C	3.16873300	-0.42853200	-3.82736000
H	3.00898300	-0.50639800	-4.90774300
C	2.07459700	-0.26979800	-2.96640300
H	1.06425300	-0.22878300	-3.39041300
C	5.17259300	-1.10488400	1.24548600
H	6.05379000	-0.78852300	0.65513000
C	4.84484600	-2.56703300	0.89972800
H	3.94322200	-2.90853200	1.43650100
H	4.66692100	-2.70341600	-0.17872500
H	5.68184500	-3.22579700	1.19196100
C	5.50976300	-0.96416300	2.73892600
H	6.31012200	-1.67227600	3.01812400
H	5.85900000	0.04789900	2.99758000
H	4.63046700	-1.18789800	3.36704600
C	5.79357000	2.00590000	0.48893300
H	6.03794600	3.08300700	0.52412900
H	6.50606700	1.49093400	1.15602100
H	5.97577700	1.65942700	-0.54090700
P	-3.34945700	-0.12231900	-0.80157300
C	-3.06418900	0.16982600	1.64899400
C	-4.19458000	0.01602100	0.80553600
C	-5.51495100	0.05007900	1.28475500
H	-6.37394400	-0.05802900	0.61498800
C	-5.70666000	0.23535800	2.66177900
H	-6.72110200	0.26587200	3.07137800
C	-4.60187000	0.38665700	3.52119800
H	-4.77559200	0.53167200	4.59269300
C	-3.28798200	0.35723400	3.02732000
H	-2.44430800	0.47993100	3.71499700
C	-2.76759600	1.49451300	-3.00719600
H	-1.86368400	1.88579200	-2.51325600
H	-2.48578300	0.57698500	-3.55131900
H	-3.09627800	2.23426700	-3.75705800
C	-3.12527900	-2.91922800	-1.37958000
H	-2.03648000	-2.79260000	-1.47043300
H	-3.33753900	-3.20779400	-0.33830500
H	-3.43466200	-3.75491000	-2.03114300
C	4.33981900	1.77619200	0.91933500
H	3.67991100	2.29940600	0.20245200
C	4.04525600	2.35668800	2.31364000
H	4.29212100	3.43303300	2.34038300
H	4.64003900	1.86476300	3.10114800
H	2.98209300	2.24268000	2.57721800
C	-5.41201300	-1.86375800	-1.70211600
H	-5.70691100	-2.69424500	-2.36696100
H	-5.71741000	-2.13083000	-0.67741800
H	-5.98525700	-0.97349000	-2.01046200
C	-3.89137200	-1.65047000	-1.77496100
H	-3.61725800	-1.38673900	-2.81533800
C	-4.30238100	2.54456400	-1.27015100
H	-4.67063900	3.27215400	-2.01404100
H	-5.10034600	2.37523000	-0.53085000
H	-3.44548800	2.99923400	-0.74998400
C	-3.89152000	1.24981700	-1.98296100
H	-4.77442500	0.84240000	-2.51356700

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