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Using fixed-charge phosphine ligands to explore coinage metal-mediated decarboxylation reactions.

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Supporting Information

Complete citation for reference 43: Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

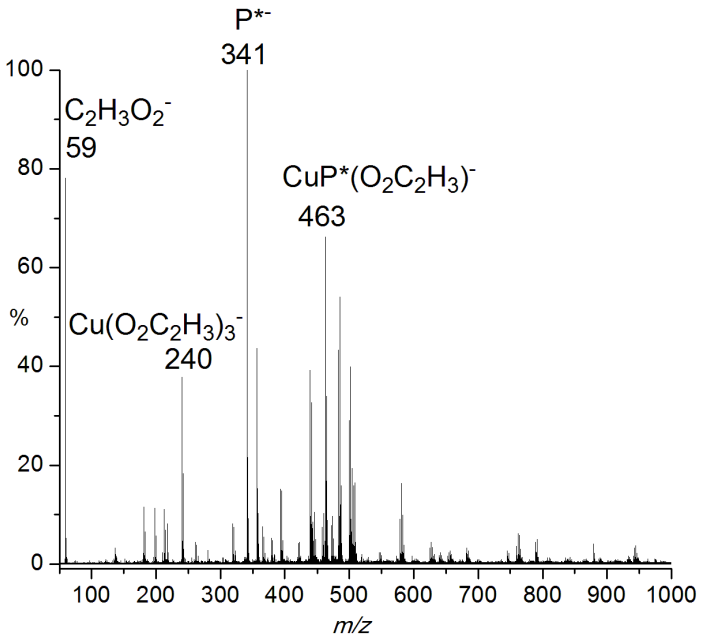


Figure S1: ESI(-)-MS of P*PPN and copper(II) acetate in methanol. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

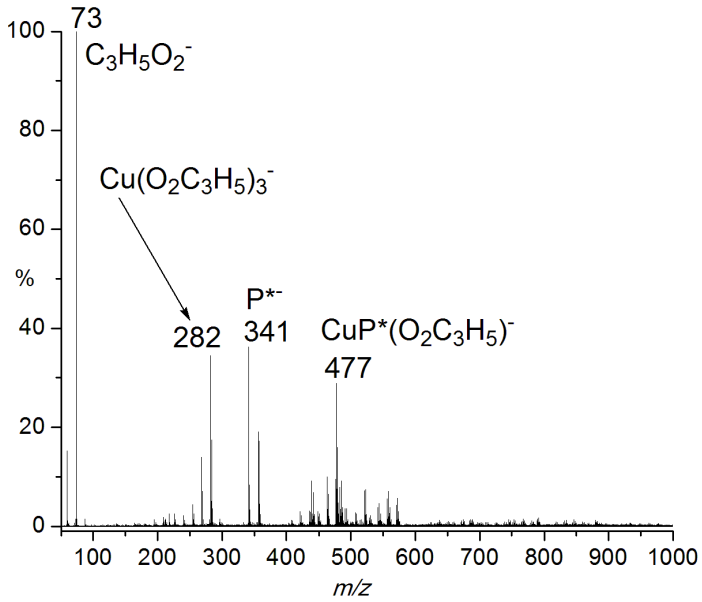


Figure S2: ESI(-)-MS of P*PPN, copper(II) acetate, and propionic acid in methanol. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

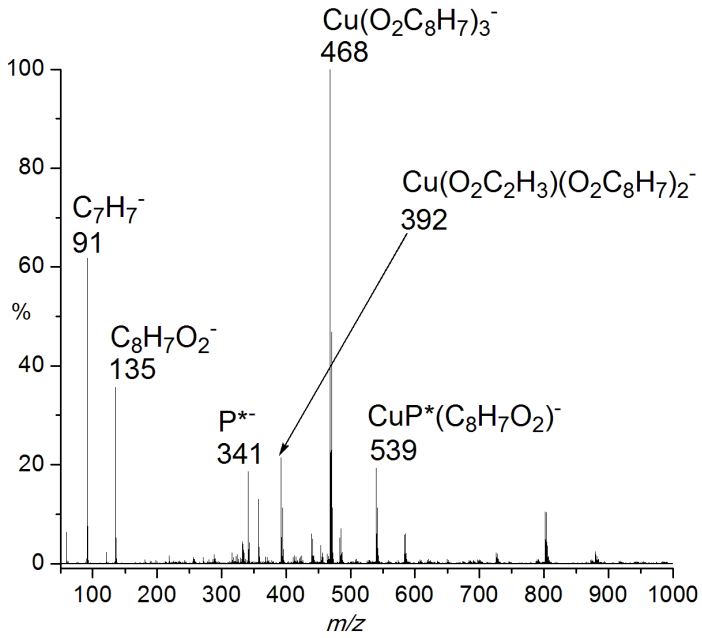


Figure S3: ESI(-)-MS of P*PPN, copper(II) acetate, and phenylacetic acid in methanol. P^{*-} = $P(C_6H_5)_2(C_6H_4SO_3)^-$.

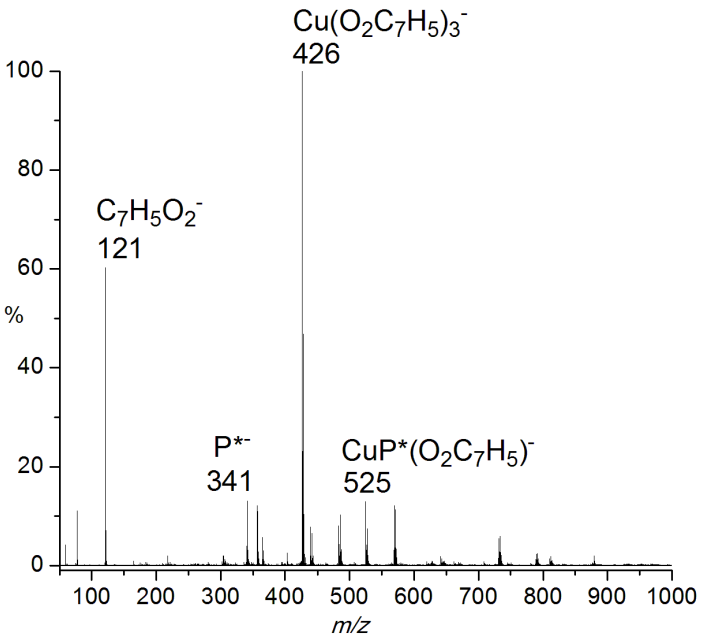


Figure S4: ESI(-)-MS of P*PPN, copper(II) acetate, and benzoic acid in methanol. P^{*-} = $P(C_6H_5)_2(C_6H_4SO_3)^-$.

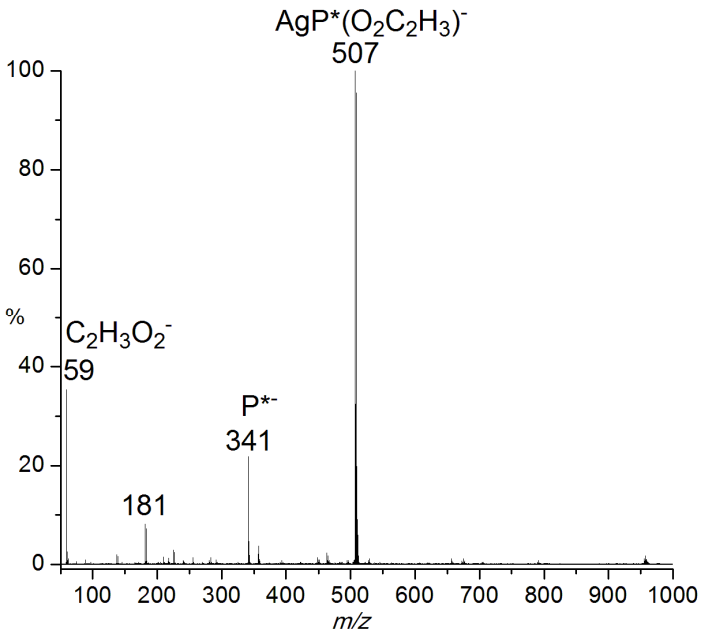


Figure S5: ESI(-)-MS of P*PPN and silver(I) acetate in methanol. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

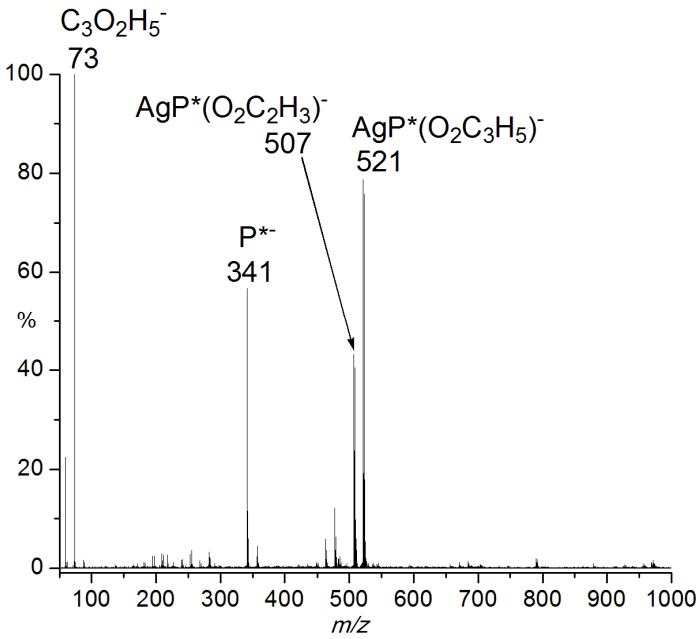


Figure S6: ESI(-)-MS of P*PPN, silver(I) acetate, and propionic acid in methanol. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

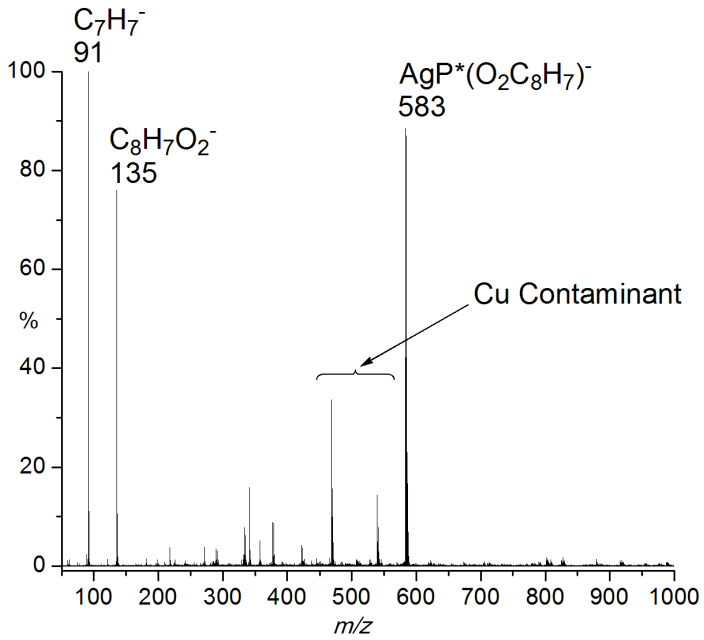


Figure S7: ESI(-)-MS of P*PPN, silver(I) acetate, and phenylacetic acid in methanol. P*- = $P(C_6H_5)_2(C_6H_4SO_3)^-$.

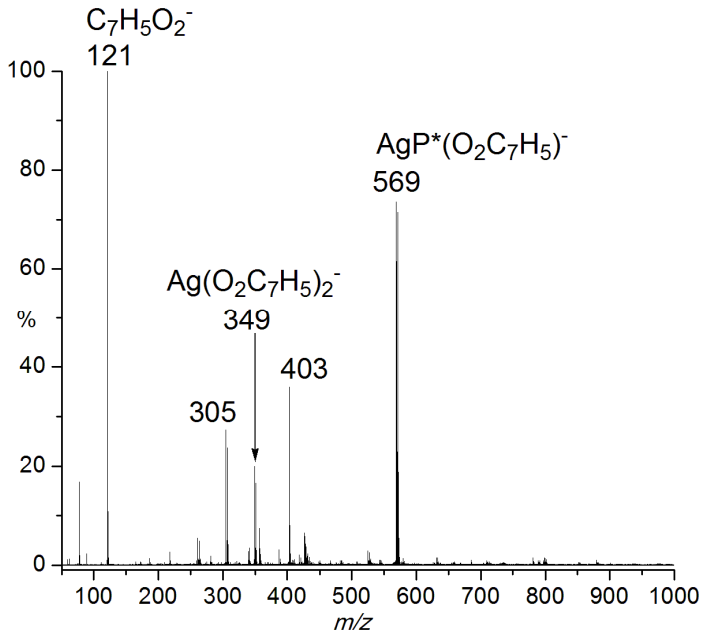


Figure S8: ESI(-)-MS of P*PPN, silver(I) acetate, and benzoic acid in methanol. P*- = $P(C_6H_5)_2(C_6H_4SO_3)^-$.

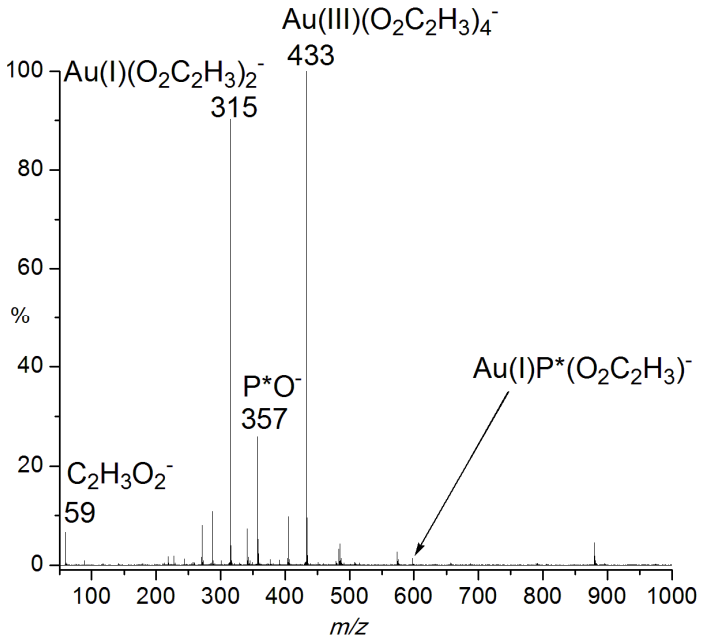


Figure S9: ESI(-)-MS of P*PPN and gold(III) acetate in methanol. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

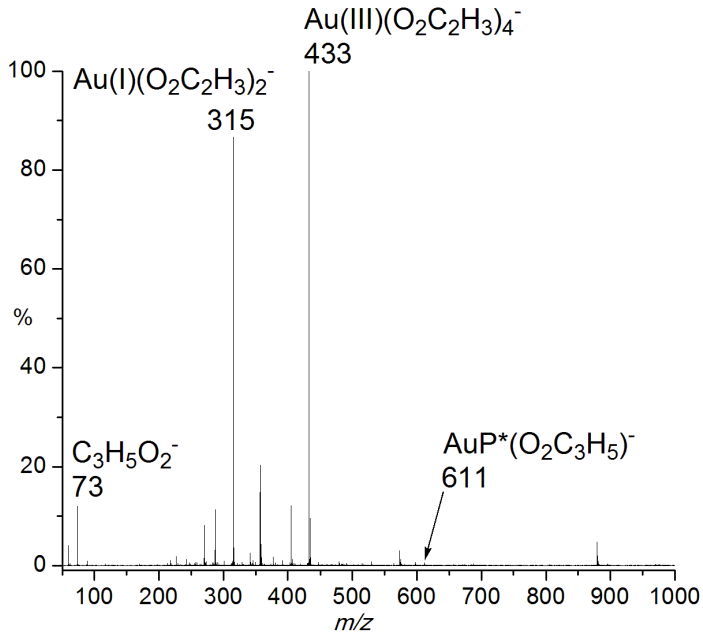


Figure S10: ESI(-)-MS of P*PPN, gold(III) acetate, and propionic acid in methanol. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

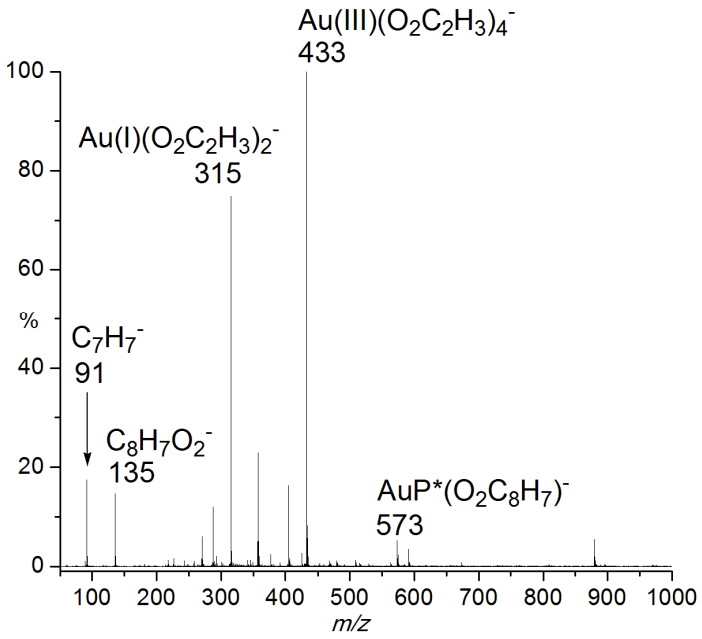


Figure S11: ESI(-)-MS of P*PPN, gold(III) acetate, and phenylacetic acid in methanol. P*$^{-}$ = $P(C_6H_5)_2(C_6H_4SO_3)^-$.

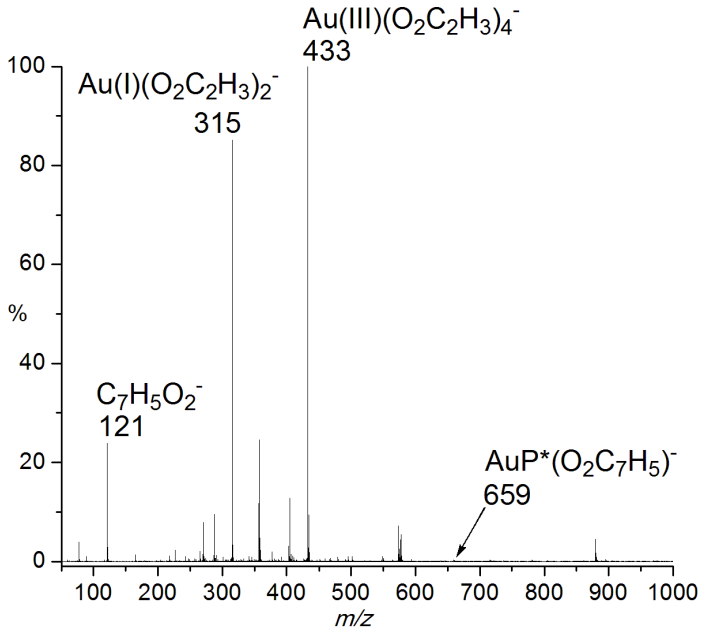


Figure S12: ESI(-)-MS of P*PPN, gold(III) acetate, and benzoic acid in methanol. P*$^{-}$ = $P(C_6H_5)_2(C_6H_4SO_3)^-$.

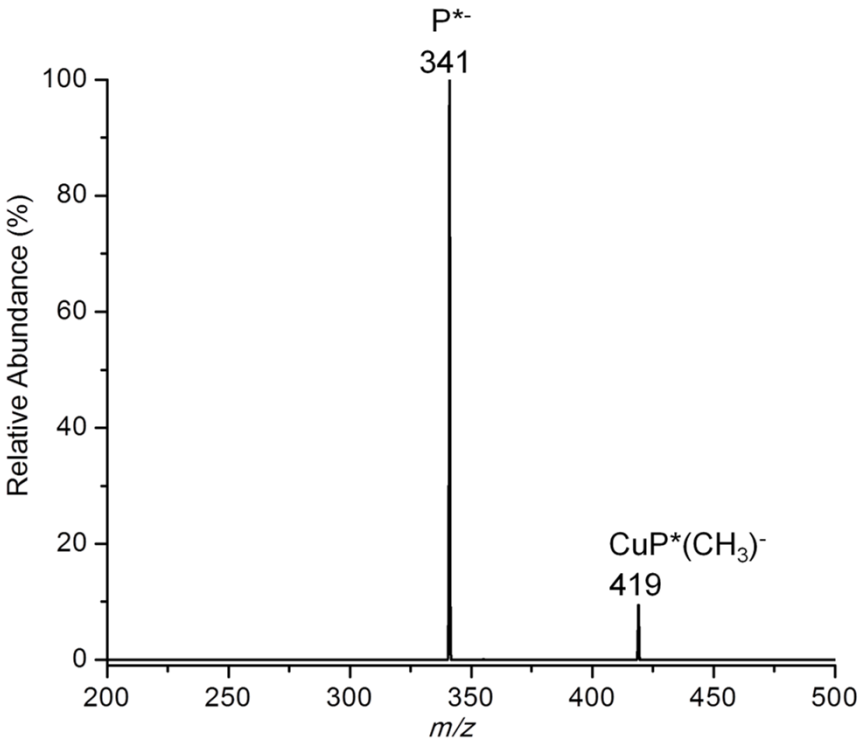


Figure S13: CID of $CuP^*(CH_3)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

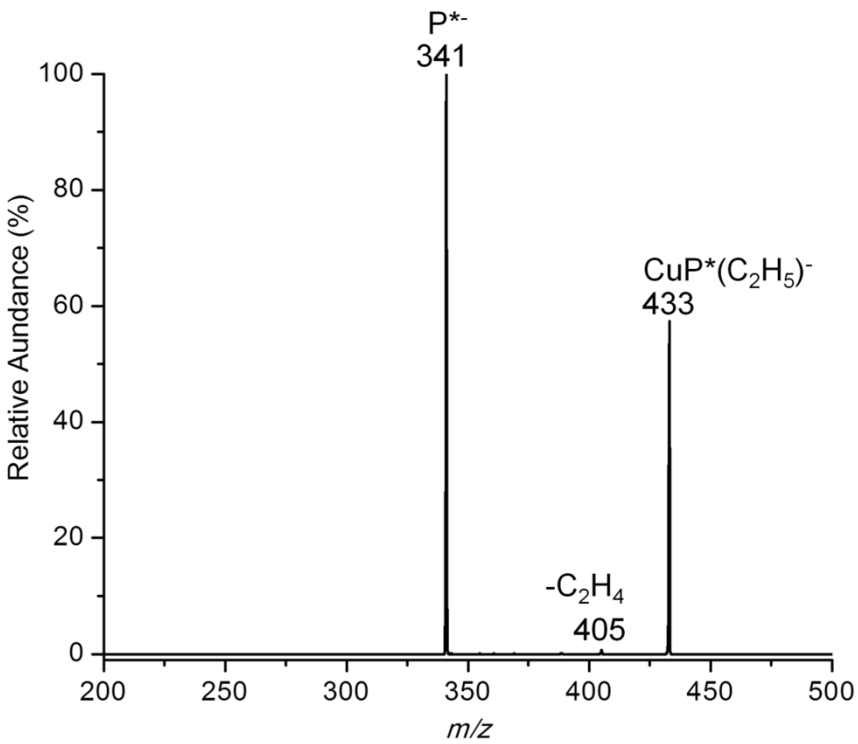


Figure S14: CID of $CuP^*(C_2H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

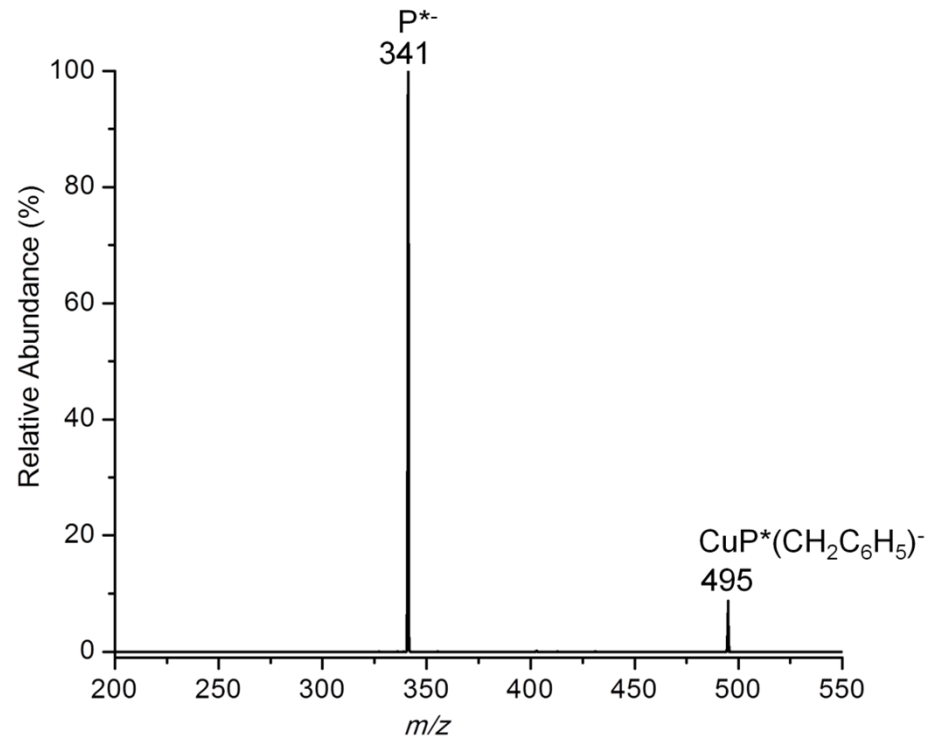


Figure S15: CID of $CuP^*(CH_2C_6H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

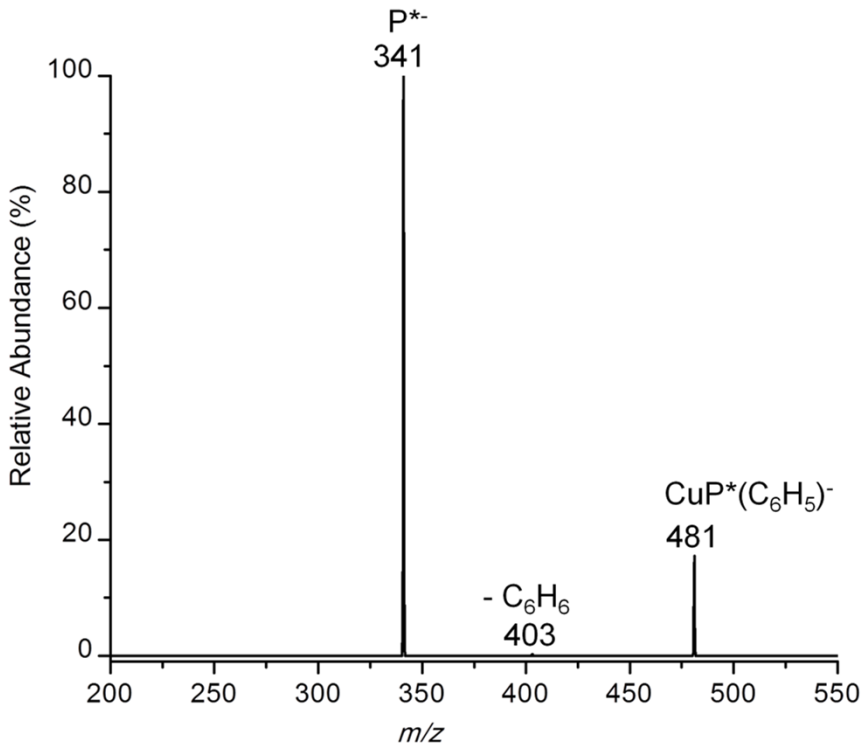


Figure S16: CID of $CuP^*(C_6H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

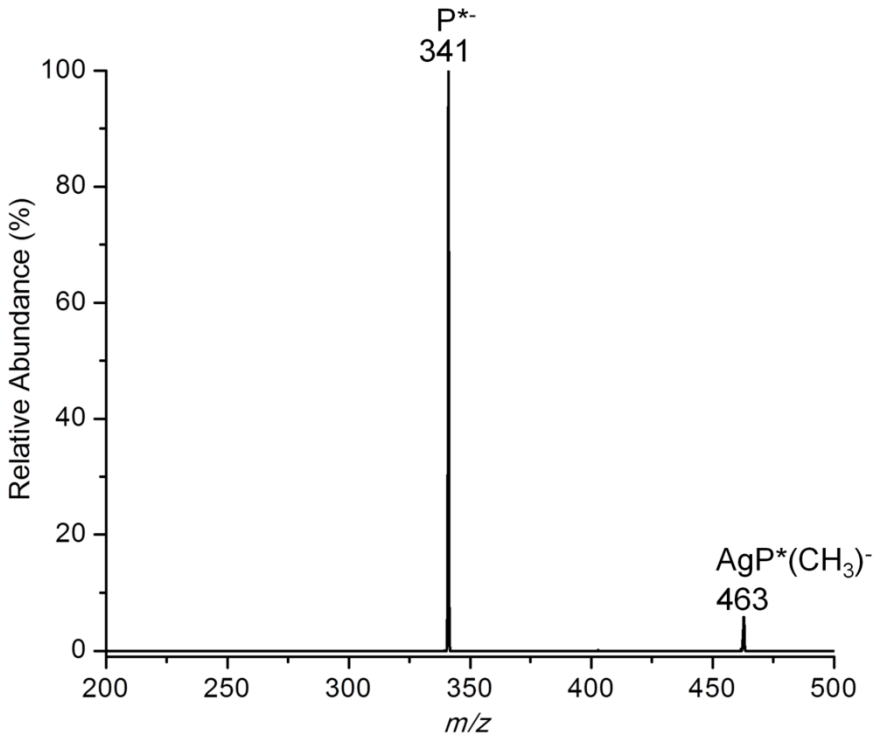


Figure S17: CID of $AgP^*(CH_3)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

Note: $AgP^*(C_2H_5)^-$ was too small to isolate for CID

Figure S18: CID of $AgP^*(C_2H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

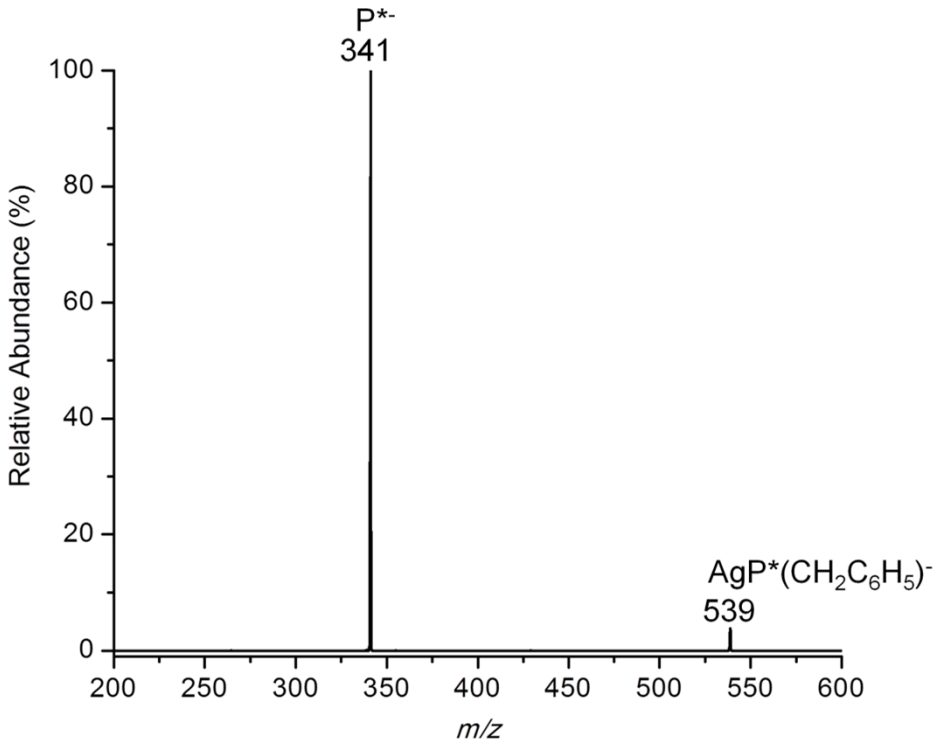


Figure S19: CID of $AgP^*(CH_2C_6H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

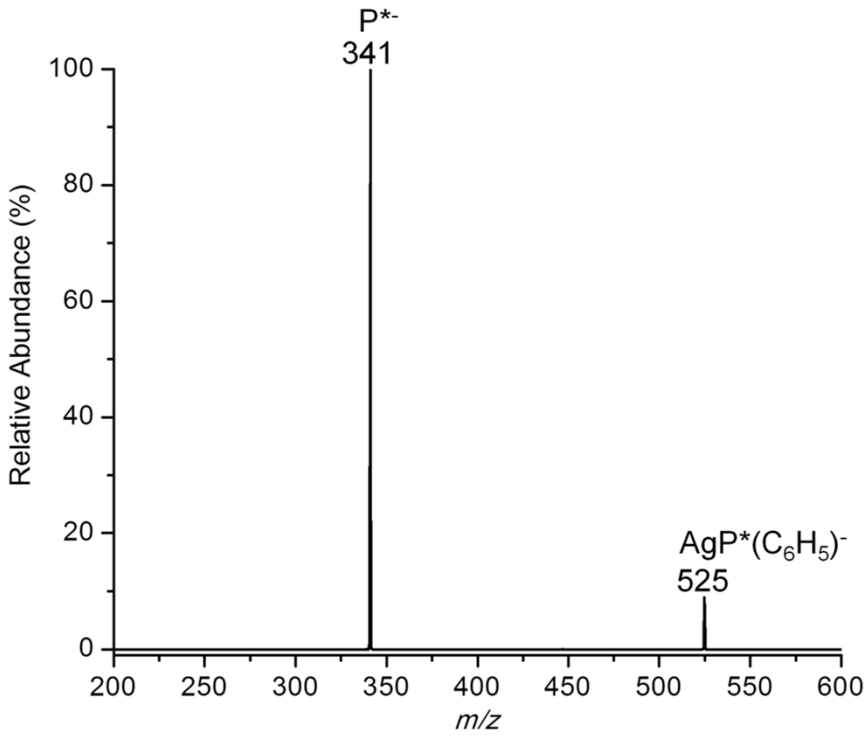


Figure S20: CID of $AgP^*(C_6H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

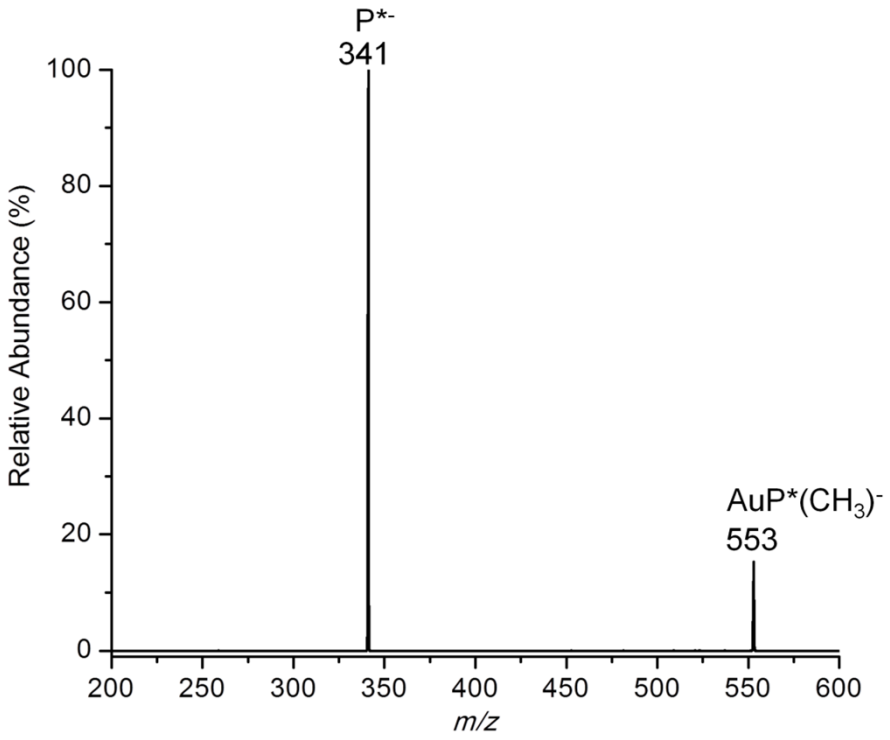


Figure S21: CID of $AuP^*(CH_3)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

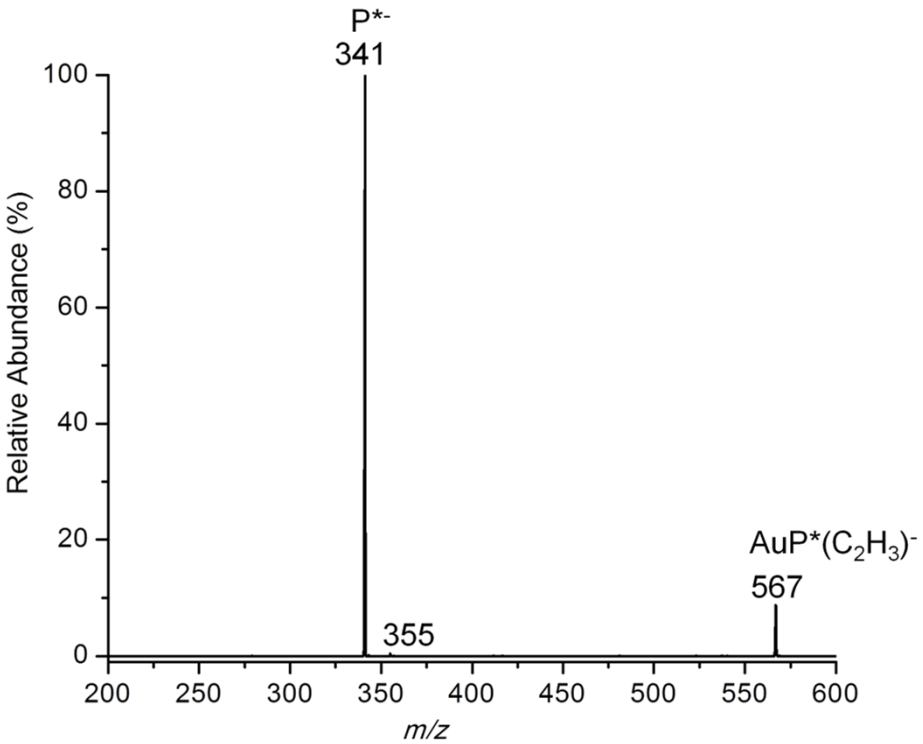


Figure S22: CID of $AuP^*(C_2H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

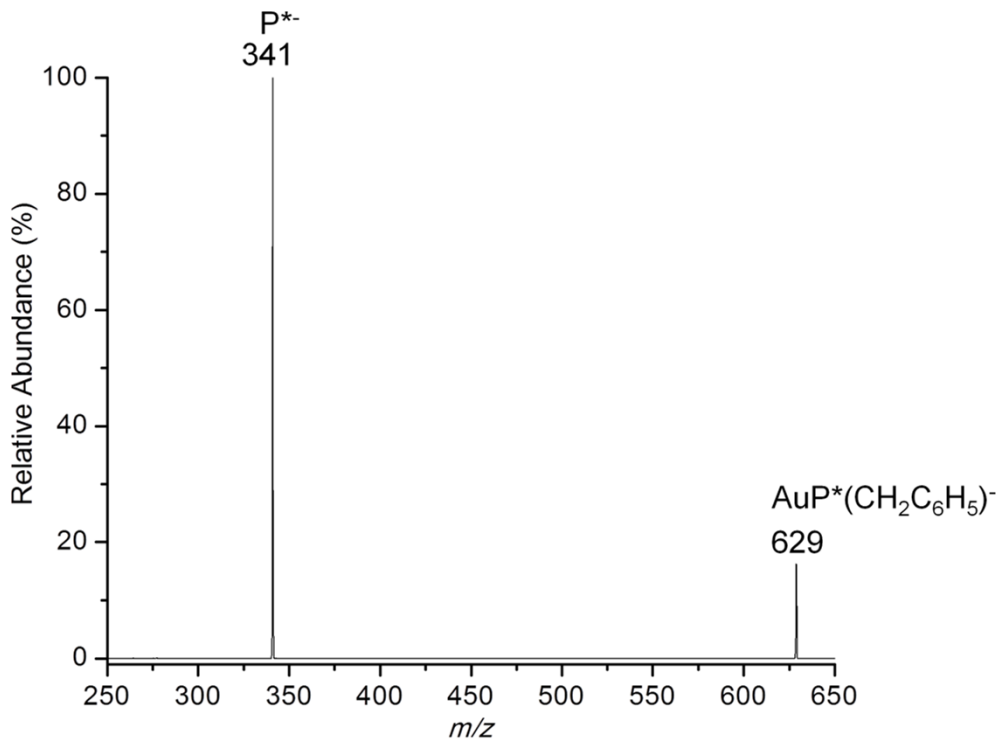


Figure S23: CID of $AuP^*(CH_2C_6H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

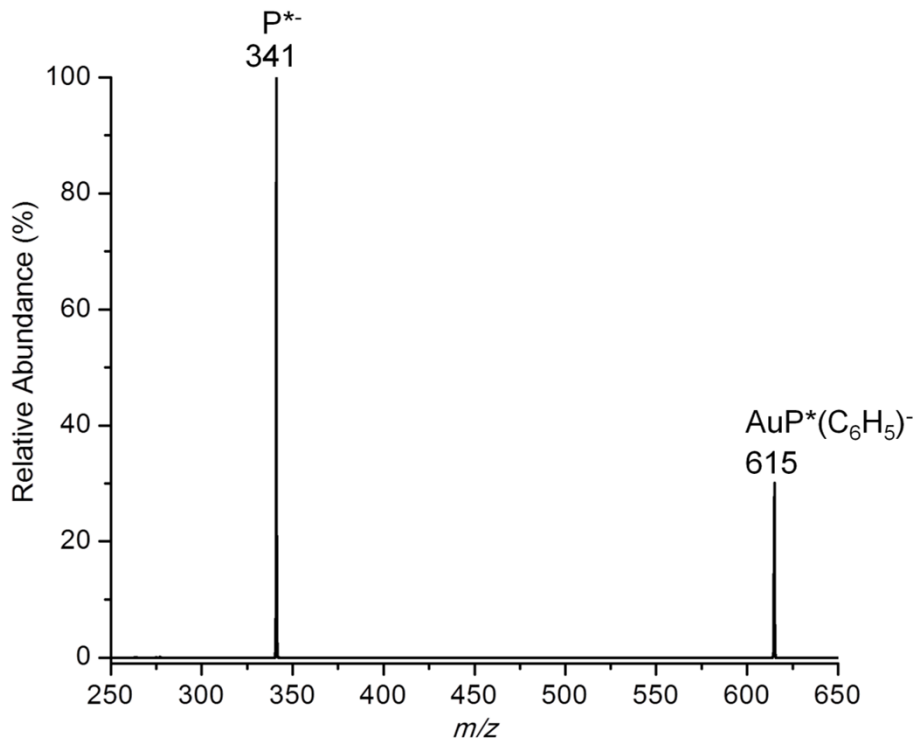


Figure S24: CID of $AuP^*(C_6H_5)^-$. $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

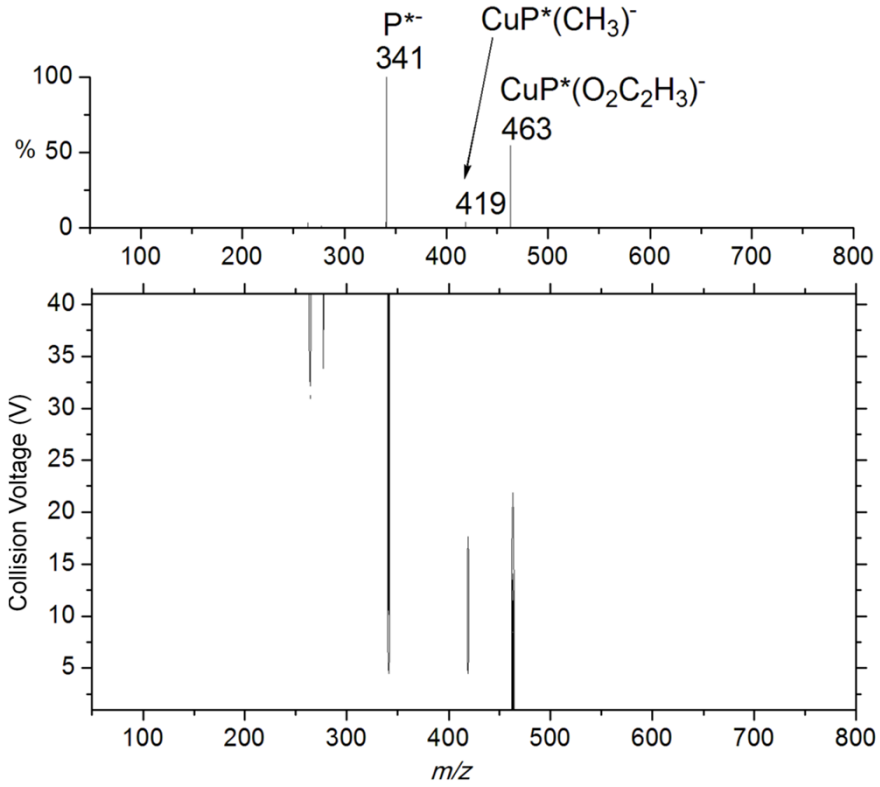


Figure S25: Energy-dependent CID of $CuP^*(O_2C_2H_3)^-$ (**1a**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

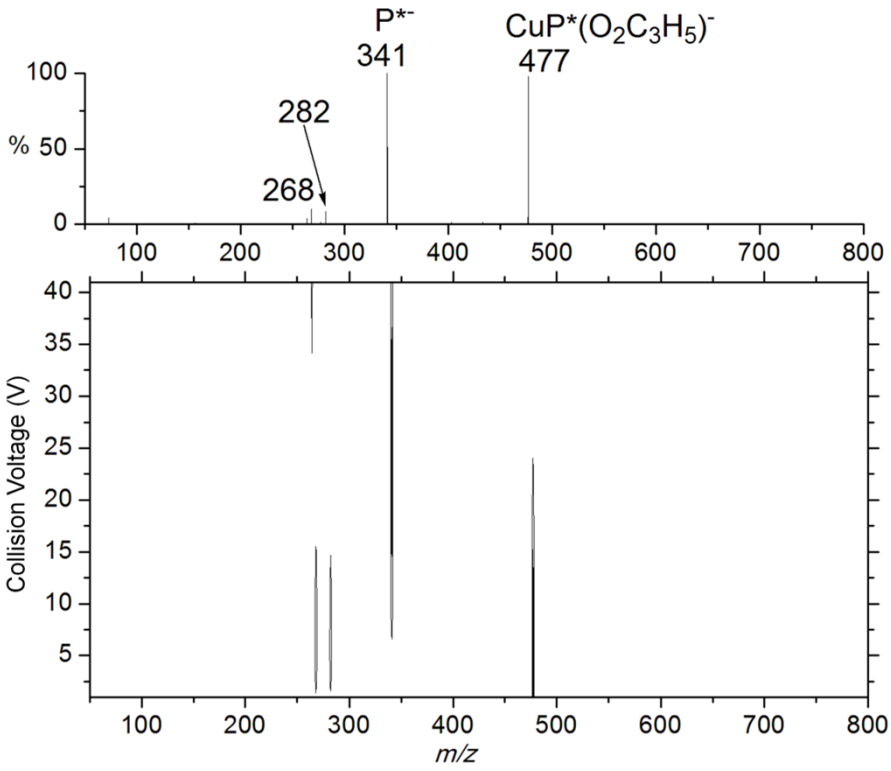


Figure S26: Energy-dependent CID of $CuP^*(O_2C_3H_5)^-$ (**2a**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

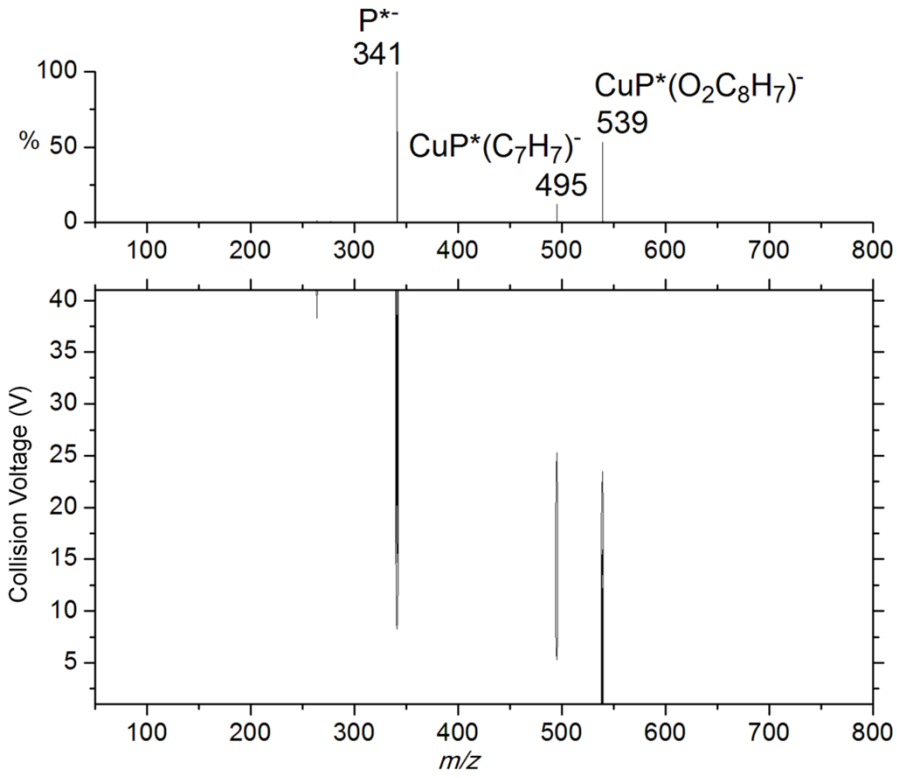


Figure S27: Energy-dependent CID of $CuP^*(O_2C_8H_7)^-$ (**3a**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

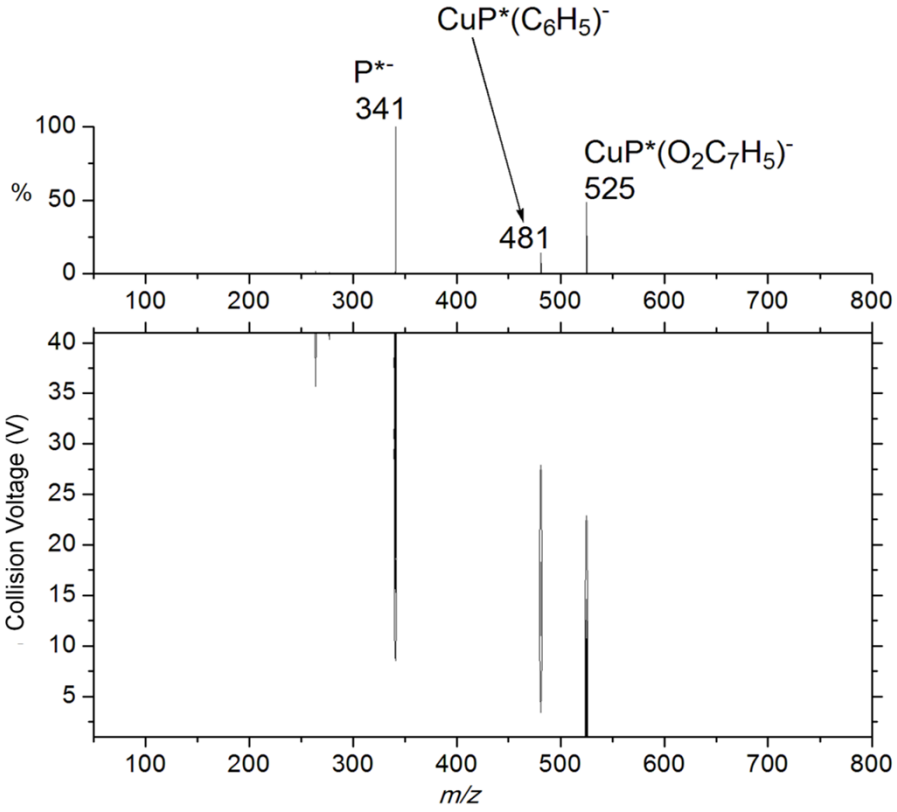


Figure S28: Energy-dependent CID of $CuP^*(O_2C_7H_5)^-$ (**4a**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

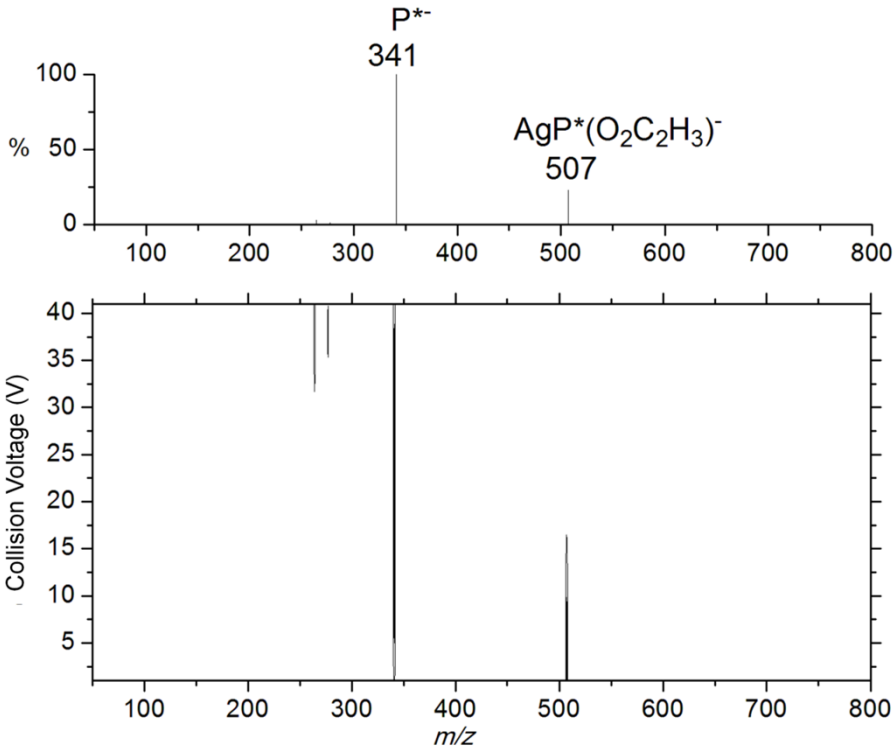


Figure S29: Energy-dependent CID of $AgP^*(O_2C_2H_3)^-$ (**1b**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

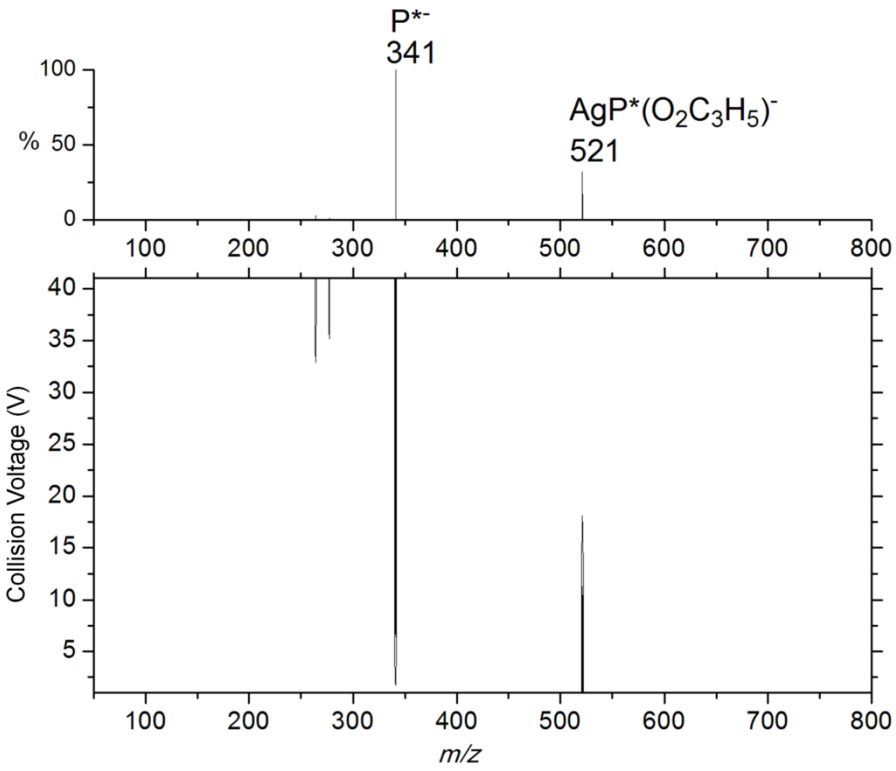


Figure S30: Energy-dependent CID of $AgP^*(O_2C_3H_5)^-$ (**2b**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

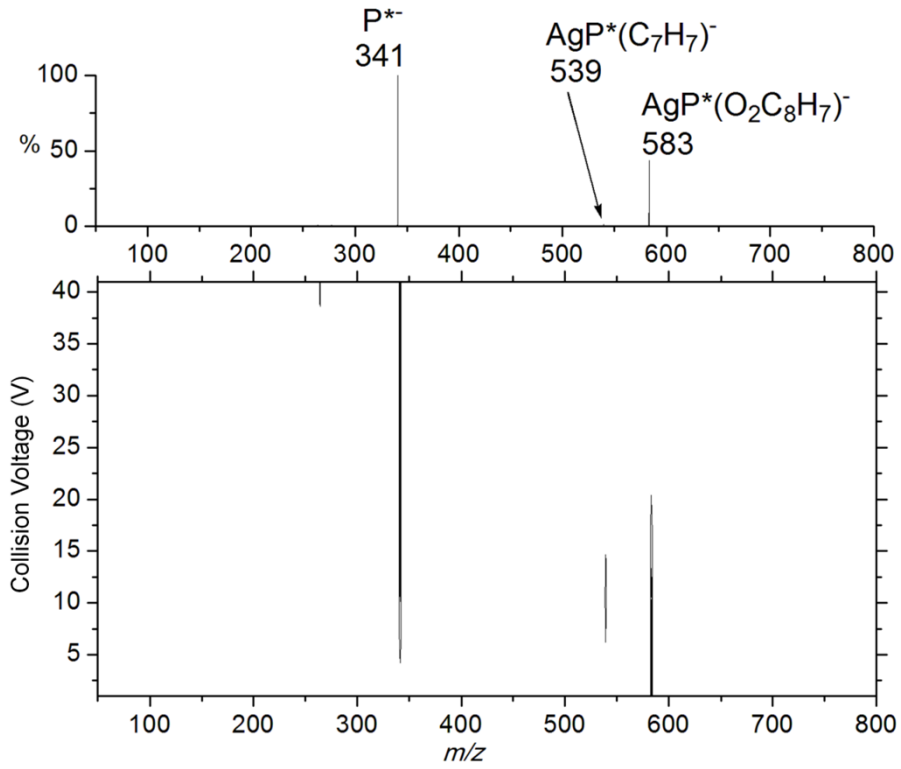


Figure S31: Energy-dependent CID of $AgP^*(O_2C_8H_7)^-$ (**3b**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

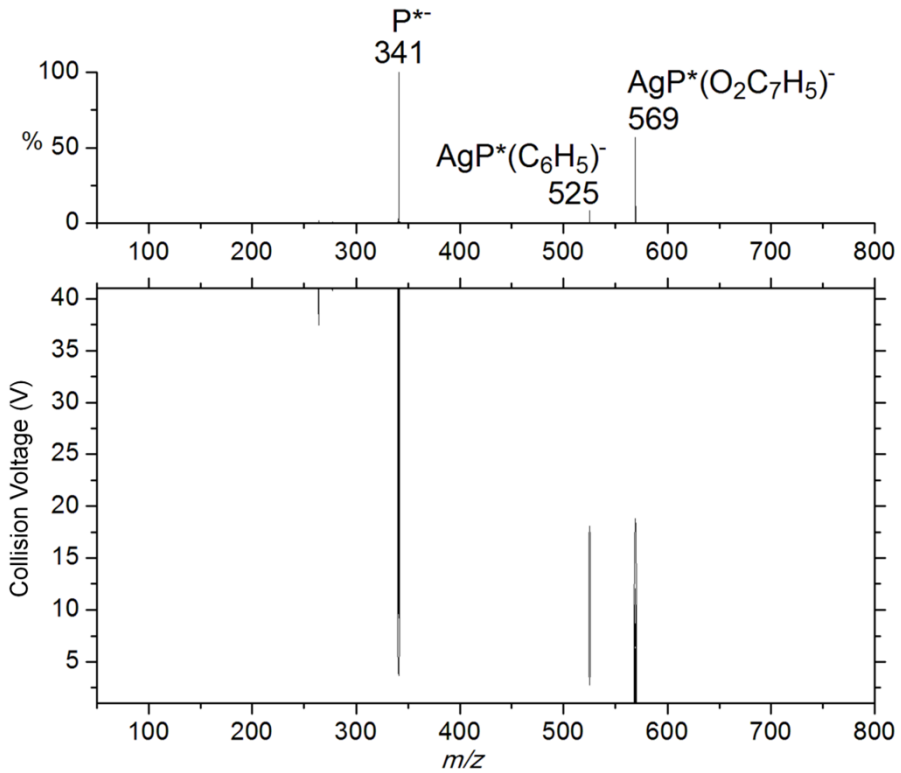


Figure S32: Energy-dependent CID of $AgP^*(O_2C_7H_5)^-$ (**4b**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

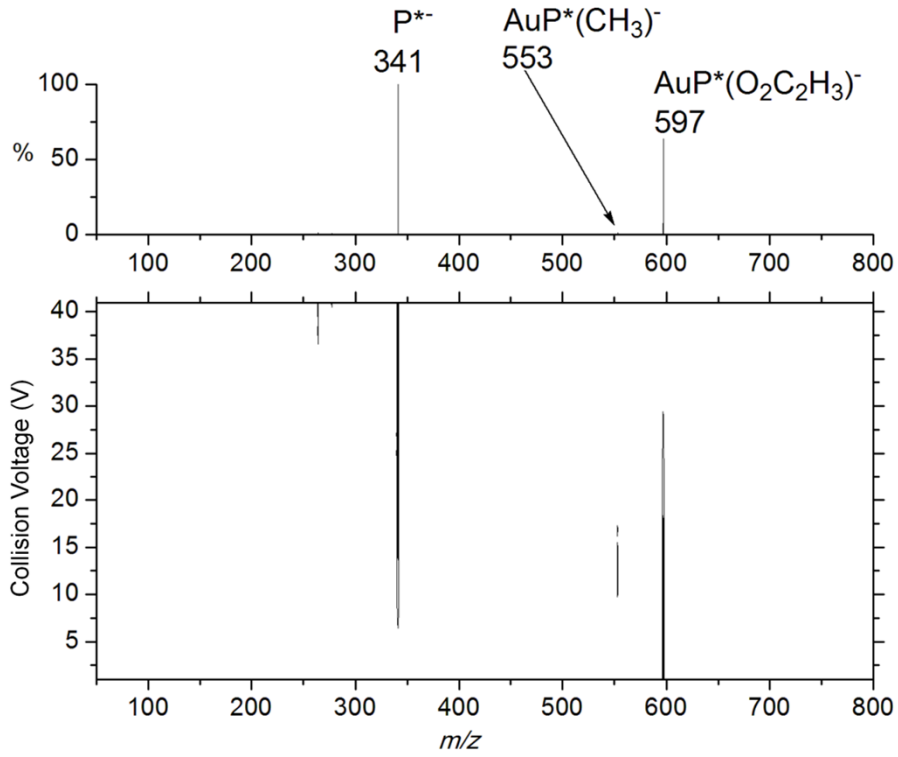


Figure S33: Energy-dependent CID of $AuP^*(O_2C_2H_3)^-$ (**1c**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

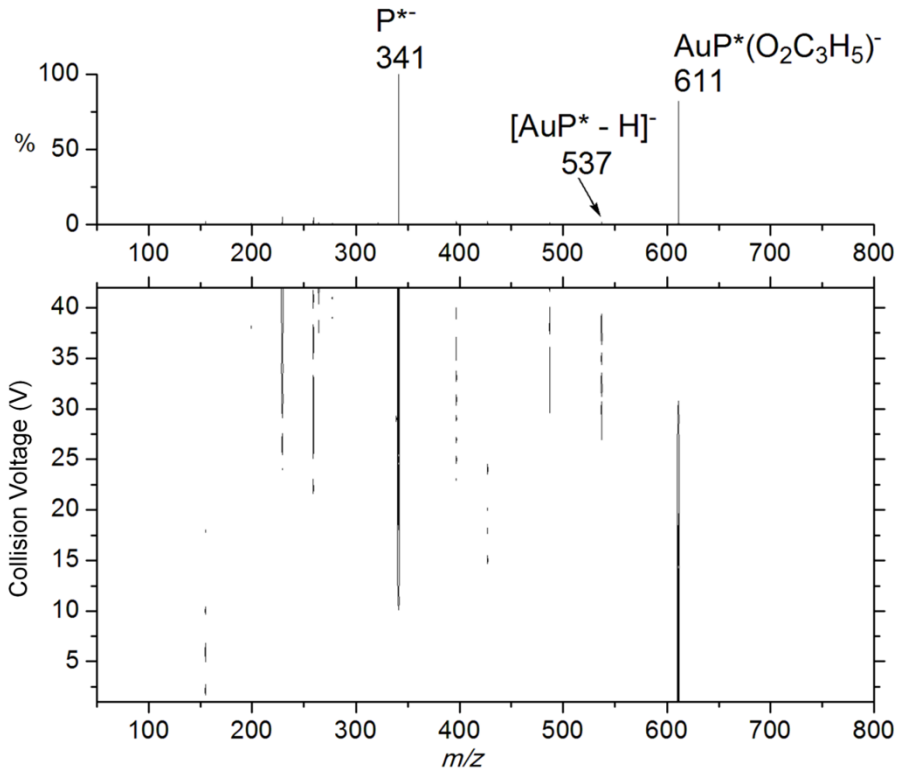


Figure S34: Energy-dependent CID of $AuP^*(O_2C_3H_5)^-$ (**2c**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

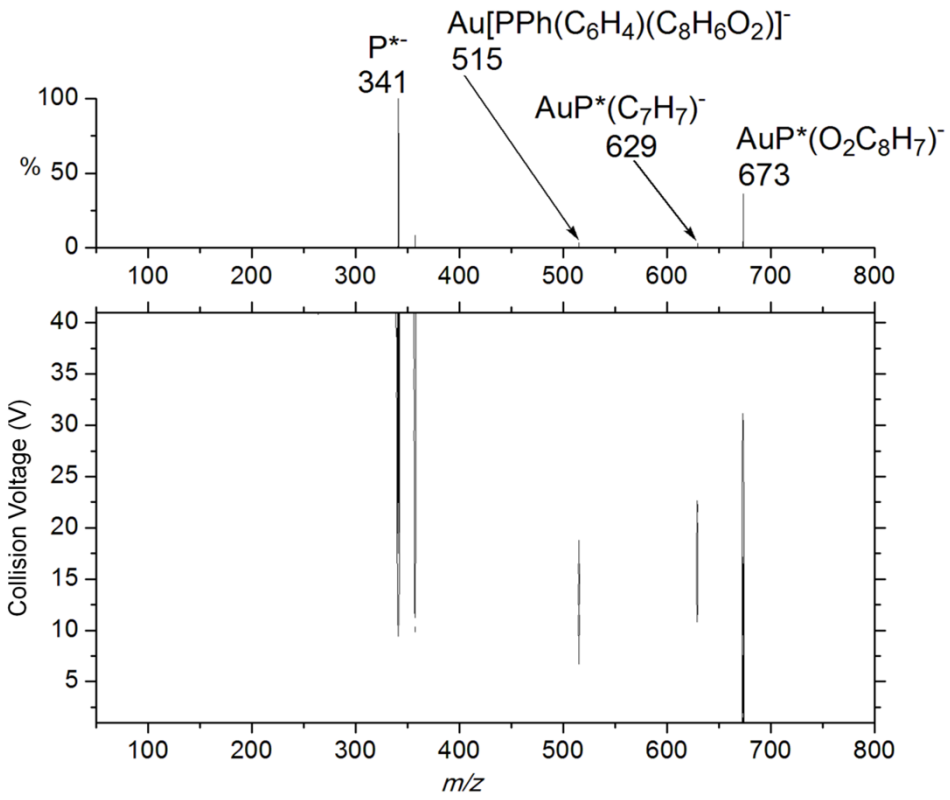


Figure S35: Energy-dependent CID of $AuP^*(O_2C_8H_7)^-$ (**3c**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

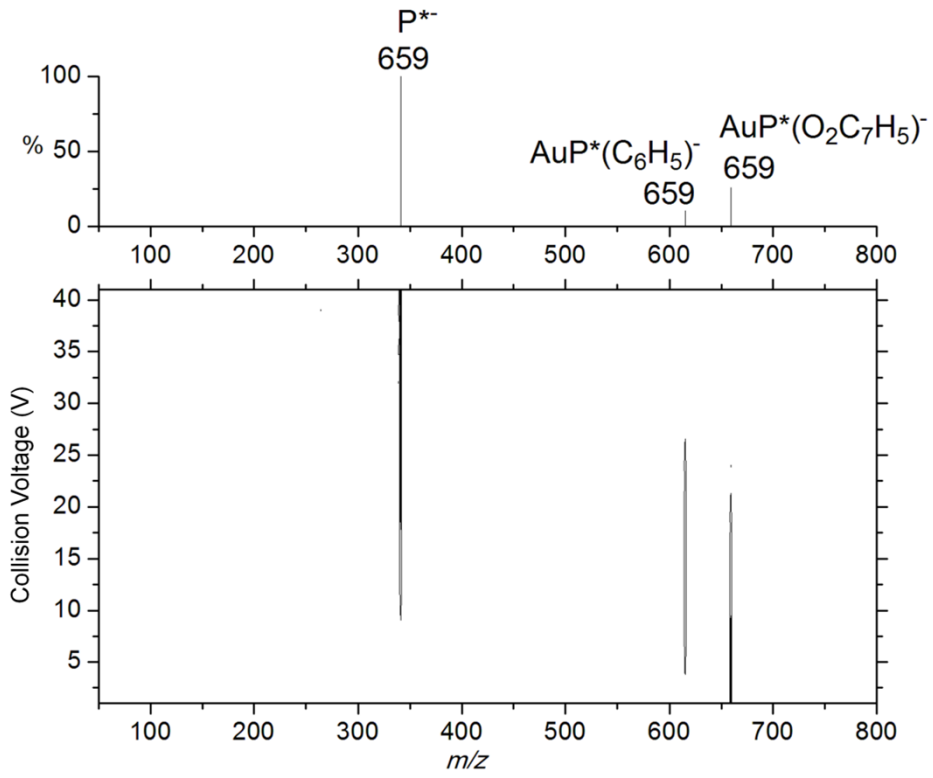


Figure S36: Energy-dependent CID of $AuP^*(O_2C_7H_5)^-$ (**4c**). $P^{*-} = P(C_6H_5)_2(C_6H_4SO_3)^-$.

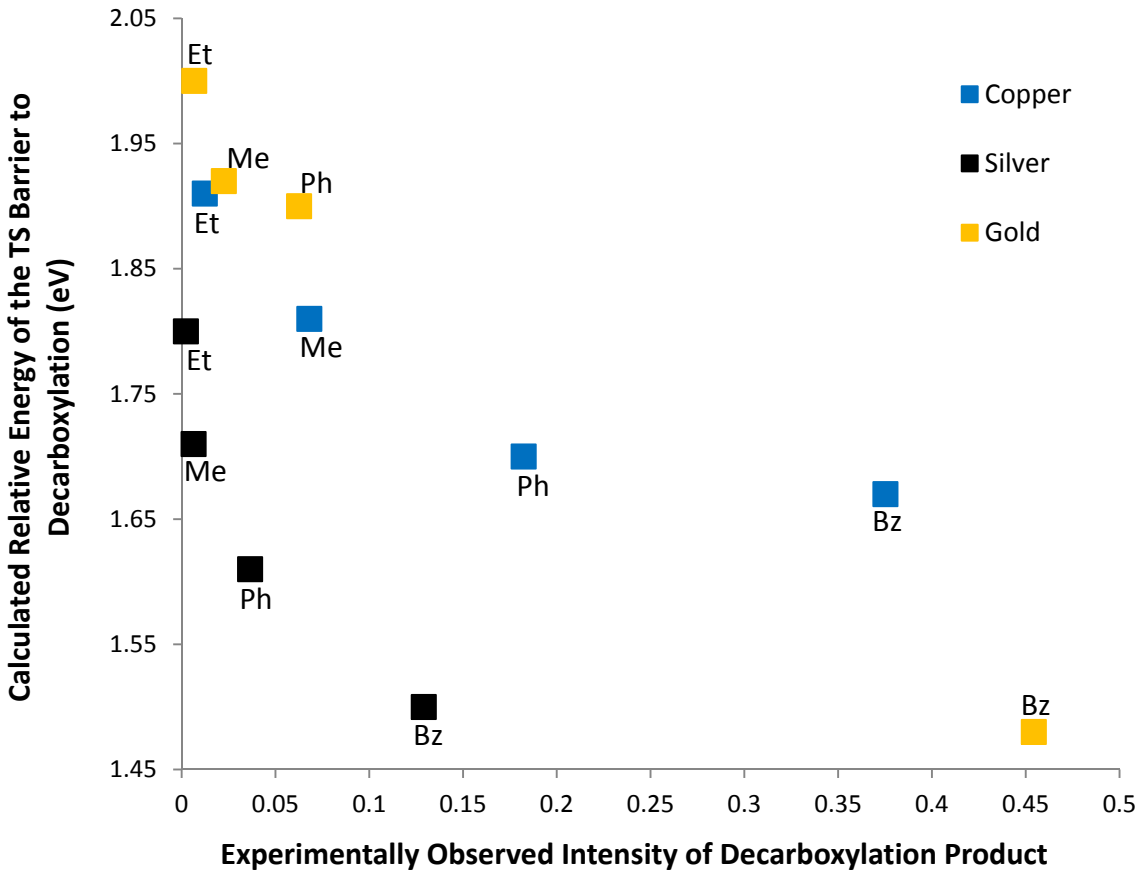
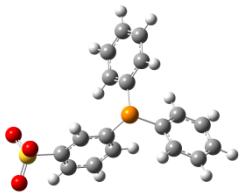


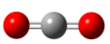
Figure S37: A comparison of the experimental ease of decarboxylation (x-axis) and the calculated transition state energy for decarboxylation (y-axis) from $[LMO_2CR]^-$ where L = $PPh_2(C_6H_4SO_3)^-$, M = Cu (blue), Ag (black) or Au (yellow) and R = Me, Et, benzyl (Bz) or Ph (see data point labels). The DFT -calculated transition state energy relative to the reactant is plotted on the y-axis. On the x-axis, the intensity of the decarboxylation fragmentation channel relative to the intensity of the reactant ion is taken from the summed energy-resolved CID experiments.



$[PPh_2C_6H_4SO_3]^-$

P	-1.09978200	-0.02168500	-1.07401900
C	-2.46397200	-1.13338600	-0.47059700
C	-2.54947900	-2.40937300	-1.05780200
C	-3.42233700	-0.78190000	0.49396000
C	-3.54691000	-3.31140900	-0.68125700
H	-1.82373700	-2.69786100	-1.81561000
C	-4.43124400	-1.67872400	0.86315300
H	-3.38175600	0.19746000	0.96208400
C	-4.49594200	-2.94727300	0.28037600
H	-3.58743100	-4.29506200	-1.14399900
H	-5.16281100	-1.38511800	1.61323800
H	-5.27873200	-3.64486300	0.56971400
C	-1.59791500	1.61703800	-0.35459900
C	-0.94420000	2.22882400	0.72640300
C	-2.63627600	2.32138800	-0.99280900
C	-1.32894600	3.50067800	1.16631500
H	-0.12504800	1.71589800	1.22131800
C	-3.03184500	3.58321600	-0.54521000
H	-3.13752400	1.87713300	-1.85108900
C	-2.37610000	4.17952400	0.53828200
H	-0.80191800	3.95978700	1.99959900
H	-3.84079600	4.10687700	-1.05041700
H	-2.67160600	5.16885800	0.88033400
C	0.32963700	-0.53066400	-0.01989000
C	1.61449600	-0.21266300	-0.49650000
C	0.20323200	-1.20765100	1.20510300
C	2.75116100	-0.54088400	0.24646600
H	1.75036300	0.28362400	-1.45408000
C	1.34510900	-1.55411600	1.93447000
H	-0.77934600	-1.47317200	1.58567800
C	2.61658000	-1.21897000	1.46135800
H	1.23946100	-2.09067700	2.87592500
H	3.51166800	-1.49159200	2.01270300
S	4.41406300	-0.04391600	-0.33713700
O	4.67082600	1.23001300	0.39632600
O	4.25383400	0.11542700	-1.81004600
O	5.29417100	-1.17360100	0.07818800

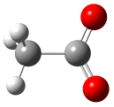
Filename: PPh3SO3
Sum of electronic and zero-point Energies = -45153.5411



CO_2

C	0.00000000	0.00024900	0.00000000
O	1.18355200	0.02374700	0.00000000
O	-1.18355200	-0.02393400	0.00000000

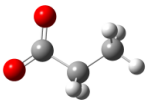
Filename: CO2
Sum of electronic and zero-point Energies = -5131.5556



$[CH_3COO]^-$

O	-0.80567200	-1.11088900	0.00001000
O	-0.70460300	1.16267700	0.00001000
C	-0.20912000	0.00116500	-0.00004800
C	1.35422800	-0.04949300	-0.00002000
H	1.72862700	-1.08042300	-0.00139300
H	1.74159300	0.47934200	-0.88234600
H	1.74132700	0.47674000	0.88399100

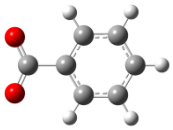
Filename: CO2Me
Sum of electronic and zero-point Energies = -6217.6038



$[CH_3CH_2COO]^-$

O	-1.75588000	-0.63955900	0.00069200
O	-0.60986500	1.32518100	-0.00039300
C	-0.70987100	0.06745200	-0.00005300
C	0.62883200	-0.74934300	-0.00089400
H	0.60528400	-1.41671100	0.87379100
H	0.60571800	-1.41387200	-0.87777700
C	1.91375200	0.08513600	0.00066500
H	2.81316300	-0.55330400	-0.00070900
H	1.95260400	0.74150800	-0.87666800
H	1.95291500	0.73793100	0.88067500

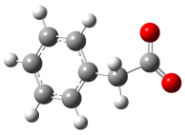
Filename: CO2Et
Sum of electronic and zero-point Energies = -7286.6586



$[PhCOO]^-$

O	-2.37493500	1.13801900	0.00008400
O	-2.37484400	-1.13804300	-0.00008000
C	-1.83368600	-0.00000400	-0.00000200
C	-0.28101300	0.00002300	-0.00000300
C	0.43770200	-1.20456300	0.00003100
C	0.43773100	1.20459000	-0.00003400
C	1.83693900	-1.20891800	0.00003600
H	-0.13402100	-2.12860900	0.00005400
C	1.83696900	1.20891300	-0.00003600
H	-0.13396700	2.12865200	-0.00005000
C	2.54443700	-0.00001100	0.00000100
H	2.37892500	-2.15459300	0.00007100
H	2.37897600	2.15457600	-0.00006200
H	3.63384300	-0.00002400	0.00000400

Filename: CO2Ph
Sum of electronic and zero-point Energies = -11434.10673

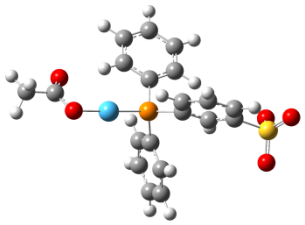


$[PhCH_2COO]^-$

O	3.03847900	-0.79776100	-0.66721300
O	2.28755500	1.31740800	-0.28188000
C	2.29175200	0.06626300	-0.14524900
C	1.20374400	-0.49759300	0.86855200
H	1.36984600	-1.57082100	1.00752700
H	1.39356000	0.00705400	1.82640900
C	-0.21885200	-0.24656300	0.44472200
C	-0.73208500	1.06269600	0.35044300
C	-1.07698200	-1.30838900	0.10843700
C	-2.04881400	1.29231000	-0.05287200
H	-0.06194300	1.89058400	0.56205000
C	-2.39733400	-1.08228500	-0.29729400
H	-0.69726900	-2.32736700	0.16145700
C	-2.89431800	0.22214300	-0.37650200
H	-2.41844600	2.31453600	-0.12268400
H	-3.03593700	-1.92686900	-0.55292000
H	-3.92075100	0.40421100	-0.69051900

Filename: CO2CH2Ph
Sum of electronic and zero-point Energies = -12503.0304

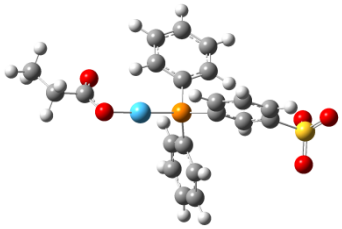
Figure S38: Cartesian coordinates and energies (eV) for $P(C_6H_5)_2(C_6H_4SO_3)$,CO_2 and $RCOO^-$ (R = Me, Et, Ph and CH_2Ph).



$[(CH_3CO_2)Cu(PPh_2C_6H_4SO_3)]^-$

Cu	-2.49052800	-0.92676200	-0.70940000
P	-0.63219400	0.05902400	-0.08492200
C	-0.83815200	0.79527600	1.59392800
C	-2.13309000	0.88939800	2.13188300
C	0.25779800	1.26309700	2.33975600
C	-2.32625400	1.45723700	3.39639200
H	-2.99241800	0.51515900	1.57765800
C	0.05752600	1.82516800	3.60179800
H	1.26814700	1.18250500	1.94983500
C	-1.23443400	1.92566100	4.13105400
H	-3.33245700	1.52235700	3.80291900
H	0.91371300	2.17852300	4.17075100
H	-1.38586800	2.36149100	5.11608900
C	-0.20046300	1.48329800	-1.17647500
C	-0.66269300	2.77640600	-0.88706400
C	0.51419000	1.26403300	-2.36581300
C	-0.40805600	3.83154700	-1.76748700
H	-1.21499300	2.96506300	0.02902500
C	0.77270400	2.32168900	-3.23970800
H	0.89436500	0.27402500	-2.60091400
C	0.31129000	3.60793400	-2.94427200
H	-0.76538600	4.82967800	-1.52573500
H	1.34897400	2.13974300	-4.14298100
H	0.51971200	4.43164100	-3.62263400
C	0.86390900	-0.99214500	-0.02582500
C	2.15670500	-0.44628900	-0.03082200
C	0.70102400	-2.38549900	0.07879100
C	3.27414600	-1.27539300	0.08273400
H	2.31897900	0.62349600	-0.12168100
C	1.82284900	-3.20967000	0.19235300
H	-0.29646200	-2.81931200	0.07358100
C	3.10815600	-2.65748500	0.19738200
H	1.69254300	-4.28647000	0.27641900
H	3.99223700	-3.28033100	0.29624200
S	4.94308800	-0.52399400	0.03842700
O	4.79110200	0.70274100	0.87225300
O	5.16361800	-0.25455100	-1.41094000
O	5.82810400	-1.57193100	0.61763800
O	-5.00876900	-0.52181200	0.46557800
O	-4.12291500	-1.73693700	-1.21299600
C	-5.11062400	-1.33492900	-0.46773900
C	-6.45933100	-1.95092200	-0.82706200
H	-7.24376900	-1.57250300	-0.16736700
H	-6.70822800	-1.71818300	-1.86913400
H	-6.40259200	-3.04278900	-0.74555800

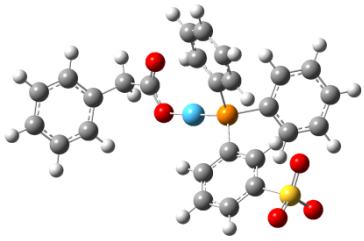
Filename: CuCO2MePPh3SO3_5
Sum of electronic and zero-point Energies = -56742.4971



$[(CH_3CH_2CO_2)Cu(PPh_2C_6H_4SO_3)]^-$

Cu	-2.26852900	-0.77380500	-0.73220500
P	-0.37269000	0.12457000	-0.08846300
C	-0.55247300	0.84147600	1.60175300
C	-1.84379800	0.98093000	2.13851400
C	0.55991400	1.25067300	2.35764400
C	-2.01672900	1.53541500	3.41182900
H	-2.71639600	0.65202900	1.57636800
C	0.37973600	1.79977600	3.62840700
H	1.56713600	1.13426800	1.96868400
C	-0.90836200	1.94555200	4.15650300
H	-3.02047200	1.63588600	3.81724400
H	1.24833800	2.10754800	4.20496600
H	-1.04424000	2.37103200	5.14830200
C	0.12057700	1.54713000	-1.15590100
C	-0.28849400	2.85350400	-0.84669400
C	0.82912700	1.31752200	-2.34694400
C	0.01218800	3.91113800	-1.70943400
H	-0.83510600	3.05026700	0.07110700
C	1.13391700	2.37743100	-3.20300000
H	1.16859100	0.31648000	-2.59716400
C	0.72523600	3.67678600	-2.88796100
H	-0.30420200	4.91922900	-1.45244600
H	1.70491800	2.18625600	-4.10771000
H	0.96964500	4.50190800	-3.55244600
C	1.07847900	-0.98838300	-0.04313100
C	2.39271600	-0.49640400	-0.03594800
C	0.85783100	-2.37529300	0.03858600
C	3.47458500	-1.37266100	0.06722900
H	2.59944900	0.56705300	-0.10887600
C	1.94431900	-3.24684600	0.14177400
H	-0.15670500	-2.76733400	0.02383100
C	3.25128100	-2.74838900	0.15914500
H	1.76940700	-4.31854500	0.20815800
H	4.10849100	-3.40881200	0.25051400
S	5.17323500	-0.69018300	0.03916000
O	5.06767100	0.53199000	0.88674900
O	5.41172900	-0.41328200	-1.40593800
O	6.01153700	-1.78032800	0.60984900
O	-4.78146900	-0.28857000	0.44644100
O	-3.93141800	-1.50645900	-1.24837100
C	-4.90810900	-1.08099400	-0.50090700
C	-6.27717800	-1.64911200	-0.88732800
H	-6.44483500	-1.40637300	-1.94551000
H	-6.19879000	-2.74422600	-0.84919000
C	-7.43735600	-1.15436200	-0.02278800
H	-7.53089800	-0.06429700	-0.07560100
H	-8.38482800	-1.60003300	-0.35386000
H	-7.28242300	-1.41376200	1.03002200

Filename: CuCO2EtPPh3SO3_4
Sum of electronic and zero-point Energies = -57811.5341

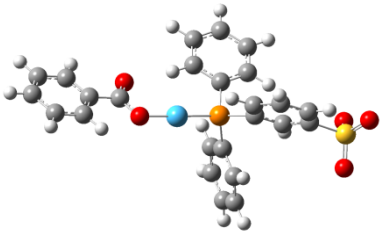


$[(PhCH_2CO_2)Cu(PPh_2C_6H_4SO_3)]^-$

Cu	-1.46912600	0.34865500	-0.82703000
P	0.58663400	0.57837700	-0.09408200
C	0.56999000	1.21583000	1.63662300
C	-0.63052100	1.73753300	2.14815400
C	1.71829600	1.19760300	2.44727100
C	-0.67475200	2.24506900	3.45146000
H	-1.53503700	1.74388500	1.54214600
C	1.66571800	1.70286100	3.74760200
H	2.65115800	0.78236100	2.07762600
C	0.47051400	2.22929100	4.25105100
H	-1.61015700	2.64312000	3.83680100
H	2.55928300	1.67851700	4.36609500
H	0.43288200	2.61842400	5.26606400
C	1.53173300	1.83981200	-1.05406000
C	1.50774000	3.19174100	-0.67773700
C	2.20445600	1.47030000	-2.23053700
C	2.15064200	4.15455400	-1.46045100
H	0.99508800	3.49573700	0.23047000
C	2.85198300	2.43400500	-3.00610500
H	2.24932800	0.42737100	-2.53070400
C	2.82568200	3.77867100	-2.62479600
H	2.13005200	5.19710200	-1.15214500
H	3.38995900	2.12736300	-3.89921400
H	3.33616100	4.52665900	-3.22646400
C	1.61841900	-0.93146200	-0.10206500
C	3.01891300	-0.87503100	-0.02822300
C	0.97650300	-2.18260700	-0.13438700
C	3.77126100	-2.04940400	0.02618900
H	3.54818900	0.07293100	-0.01049800
C	1.73494300	-3.35428000	-0.07796900
H	-0.10789600	-2.23754500	-0.19954200
C	3.12967600	-3.29020700	0.00463600
H	1.23440700	-4.31993400	-0.09872500
H	3.73529900	-4.18983300	0.06170700
S	5.59757700	-1.93130400	0.08086200
O	5.84136600	-0.76056300	0.97142000
O	5.97229400	-1.70496000	-1.34402500
O	6.02864900	-3.24398800	0.63551200
O	-3.75056400	1.61488800	0.27570600
O	-3.26377000	0.19382400	-1.40783200
C	-4.07795400	0.89683000	-0.68049200
C	-5.55939300	0.77190900	-1.08463400
H	-6.08843500	1.64989400	-0.70366200
H	-5.61825900	0.77181500	-2.17881900
C	-6.19222400	-0.49307200	-0.53725000
C	-6.00824000	-1.72784000	-1.17981700
C	-6.95949900	-0.45998800	0.63654200
C	-6.57796300	-2.89472000	-0.66481800
H	-5.40072300	-1.77018900	-2.08024300
C	-7.53083500	-1.62615700	1.15564300
H	-7.10226900	0.48783000	1.15096300
C	-7.34349700	-2.84918500	0.50556100
H	-6.42141000	-3.84176000	-1.17661500
H	-8.12045100	-1.57774800	2.06858500
H	-7.78660100	-3.75771600	0.90688600

Filename: CuCO2CH2PhPPh3SO3_3
Sum of electronic and zero-point Energies = -63027.6951

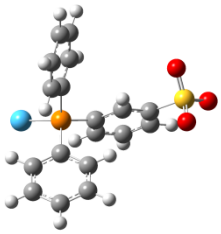
Figure S39: Cartesian coordinates and energies (eV) for $[(RCO_2)Cu(PPh_2C_6H_4SO_3)]^-$, R = Me, Et, Ph and CH_2Ph.



$[(PhCO_2)Cu(PPh_2C_6H_4SO_3)]^-$

Cu	1.64542000	-0.48645100	0.25042000
P	-0.39685600	0.30001900	0.09345300
C	-0.45446900	1.68335000	-1.12511800
C	0.75737600	2.24067900	-1.56752700
C	-1.67028900	2.19156000	-1.61456900
C	0.74853900	3.30216300	-2.47945200
H	1.70937800	1.84774800	-1.21456000
C	-1.67112900	3.24851400	-2.52655500
H	-2.61692200	1.76264000	-1.29952000
C	-0.46258900	3.80714700	-2.95845300
H	1.69250000	3.72325300	-2.81642500
H	-2.61772700	3.62920300	-2.90149300
H	-0.46753000	4.62837200	-3.67164400
C	-0.97582700	1.04179100	1.68096500
C	-0.76372200	2.40116300	1.95781800
C	-1.54711200	0.22419500	2.67014300
C	-1.12315300	2.93384400	3.19889200
H	-0.32536600	3.04885100	1.20403300
C	-1.91135200	0.76127800	3.90627400
H	-1.73447900	-0.82691500	2.47025800
C	-1.69911700	2.11673400	4.17504000
H	-0.96015700	3.99063200	3.39626400
H	-2.37550600	0.12051900	4.65127700
H	-1.98970000	2.53449000	5.13581400
C	-1.68824900	-0.89820600	-0.39750800
C	-3.05077700	-0.65861100	-0.16268400
C	-1.29715600	-2.06714800	-1.07554100
C	-4.01458700	-1.56385200	-0.61049800
H	-3.38646300	0.22776300	0.36713000
C	-2.26613500	-2.96875200	-1.52125300
H	-0.24291900	-2.26669500	-1.25443200
C	-3.62338800	-2.71809700	-1.29273900
H	-1.96004400	-3.86997800	-2.04811900
H	-4.39241900	-3.40107000	-1.64124800
S	-5.77838000	-1.22704700	-0.25329100
O	-5.90785200	0.23613400	-0.50925200
O	-5.92078800	-1.61198100	1.17961200
O	-6.51502500	-2.09994700	-1.20822900
O	3.97429000	0.82932000	-0.61924100
O	3.42502300	-1.11548200	0.37770400
C	4.27597400	-0.26690700	-0.11588100
C	5.72461600	-0.69420100	-0.04692700
C	6.09304800	-1.92548600	0.51427400
C	6.71964500	0.15425700	-0.55293800
C	7.43753300	-2.30243100	0.56804600
H	5.31479800	-2.57396500	0.90300100
C	8.06362900	-0.22157200	-0.49950800
H	6.41679500	1.10358600	-0.98388800
C	8.42607200	-1.45167100	0.06139600
H	7.71448300	-3.25946900	1.00483800
H	8.82873300	0.44317100	-0.89475800
H	9.47281100	-1.74538100	0.10321400

Filename: CuCO2PhPPh3SO3_4
Sum of electronic and zero-point Energies = -61958.7880

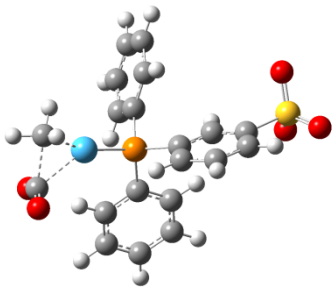


$[Cu(PPh_2C_6H_4SO_3)]^-$

P	1.25514900	-0.00528000	0.58649900
C	1.87917500	-1.17536100	-0.67473800
C	3.25203600	-1.45893500	-0.75858200
C	0.98637400	-1.77276100	-1.58124200
C	3.73270900	-2.32159600	-1.74570400
H	3.94958800	-1.00915700	-0.05404500
C	1.47444100	-2.63527400	-2.56571600
H	-0.07996700	-1.57465500	-1.52570800
C	2.84265000	-2.90978100	-2.64997500
H	4.79603400	-2.53746200	-1.80387600
H	0.77823500	-3.09294400	-3.26264200
H	3.21462200	-3.58558800	-3.41526400
C	1.21958600	1.66092700	-0.16226500
C	1.97074000	1.95712600	-1.31100600
C	0.44857700	2.66684300	0.44765100
C	1.94211200	3.24683600	-1.84700700
H	2.55886900	1.18597100	-1.79913100
C	0.42063200	3.94962500	-0.09826600
H	-0.15775500	2.44421600	1.32128000
C	1.16839600	4.24184400	-1.24388100
H	2.51270200	3.46696100	-2.74498100
H	-0.20076300	4.71329000	0.36014500
H	1.13684700	5.23990300	-1.67192000
C	-0.43169900	-0.46111600	1.04731300
C	-1.49576100	-0.06596800	0.22415100
C	-0.66888700	-1.28582600	2.16497000
C	-2.78904200	-0.51417200	0.49661400
H	-1.34571800	0.58312700	-0.63347500
C	-1.96869700	-1.70874900	2.44008400
H	0.15185200	-1.59674000	2.80953800
C	-3.02759400	-1.32936200	1.60368600
H	-2.15813800	-2.33645200	3.30722200
H	-4.04648400	-1.65191200	1.79760400
S	-4.11208800	-0.04255900	-0.68151900
O	-3.69357300	-0.77444900	-1.90975000
O	-3.96471900	1.43500300	-0.76850900
O	-5.35587200	-0.53037900	-0.03784300
Cu	2.55983100	-0.03571000	2.35980600

Filename: CuPPh3SO3
Sum of electronic and zero-point Energies = -50520.7214

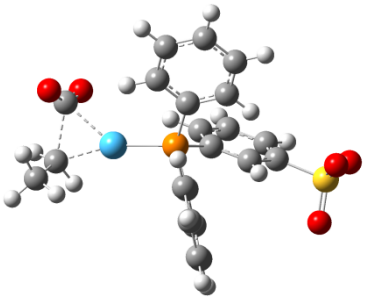
Figure S39 (cont'd): Cartesian coordinates and energies (eV) for $[(RCO_2)Cu(PPh_2C_6H_4SO_3)]^-$, R = Me, Et, Ph and CH_2Ph, and for $[Cu(PPh_2C_6H_4SO_3)]^-$.



TS $[(CH_3CO_2)Cu(PPh_2C_6H_4SO_3)]^-$ → $[(CH_3)Cu(PPh_2C_6H_4SO_3)]^-$
(-339 cm^{-1})

Cu	2.56740100	-0.91793500	-0.83840800
O	4.83858600	-2.71865800	0.30074300
C	4.61758600	-1.62136200	-0.15310200
O	4.81440200	-0.42737700	0.05835600
C	3.90352300	-1.94657800	-2.01446500
H	3.39800000	-1.30905100	-2.77089600
H	4.95860500	-1.91421800	-2.29848100
H	3.54823300	-2.97760500	-2.08113300
P	0.74501200	0.10442200	-0.08089800
C	0.28610200	1.51000300	-1.18609900
C	0.71067900	2.81816500	-0.90817900
C	-0.41744000	1.25845100	-2.37608200
C	0.43014800	3.85660900	-1.80091800
H	1.25240300	3.03221300	0.00852800
C	-0.70240400	2.29919100	-3.26156400
H	-0.77046400	0.25596300	-2.60119000
C	-0.27777400	3.60087900	-2.97781800
H	0.75776600	4.86686900	-1.56785000
H	-1.27102000	2.09235000	-4.16428800
H	-0.50693800	4.41145400	-3.66515100
C	0.97998200	0.86736000	1.58102200
C	-0.11090400	1.27840400	2.36649300
C	2.28663800	1.04444000	2.06525100
C	0.10671700	1.86666400	3.61382200
H	-1.12939300	1.13417000	2.01836200
C	2.49766300	1.63674000	3.31511200
H	3.14034900	0.71363900	1.47842200
C	1.41031000	2.04891900	4.08921600
H	-0.74533400	2.17642500	4.21345500
H	3.51335500	1.76400000	3.68126600
H	1.57527700	2.50339600	5.06345700
C	-0.74548000	-0.94934800	0.02821900
C	-0.57649400	-2.33748400	0.18421000
C	-2.03927100	-0.40702600	0.01185500
C	-1.69502000	-3.15937900	0.33682300
H	0.42194700	-2.76909200	0.19151000
C	-3.15350700	-1.23489200	0.16260700
H	-2.20409100	0.65866100	-0.11584800
C	-2.98233000	-2.61096800	0.32780000
H	-1.56073000	-4.23159200	0.46188200
H	-3.86423700	-3.23192200	0.45412700
S	-4.82330600	-0.48629100	0.10657400
O	-5.03002700	-0.20970400	-1.34340500
O	-5.71199300	-1.53760200	0.67325500
O	-4.67884100	0.73660000	0.94739100

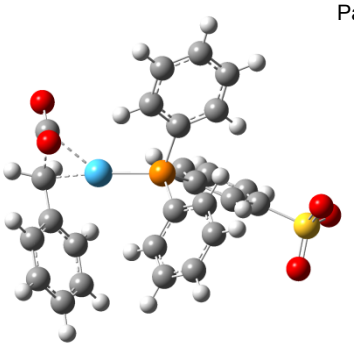
Filename: TS_CuCO2MePPh3SO3_3
Sum of electronic and zero-point Energies = -56740.6863



TS $[(CH_3CH_2CO_2)Cu(PPh_2C_6H_4SO_3)]^-$ → $[(CH_3CH_2)Cu(PPh_2C_6H_4SO_3)]^-$
(-299 cm^{-1})

Cu	2.45478400	-0.66593700	-0.85843100
O	3.58691000	-2.84411300	-0.19647600
C	4.23799600	-1.80551300	-0.23824000
O	5.09084000	-1.19633800	0.37804700
C	4.09557200	-0.96207400	-2.08265100
H	4.67763200	-1.84201300	-2.37149400
H	3.22694900	-1.00419000	-2.77852000
P	0.59431600	0.13852500	0.05588300
C	0.17023700	1.79704200	-0.63249500
C	0.58680000	2.97350600	0.00923300
C	-0.49312000	1.89133500	-1.86750300
C	0.33822100	4.22092700	-0.57041400
H	1.09670200	2.92067800	0.96688600
C	-0.74638000	3.13913100	-2.43985100
H	-0.84055900	0.99412300	-2.37195100
C	-0.32983600	4.30738700	-1.79440800
H	0.65888900	5.12417400	-0.05695500
H	-1.28477000	3.19521900	-3.38216000
H	-0.53469900	5.27852000	-2.23811700
C	0.75600600	0.40738900	1.87199000
C	-0.36428400	0.68310400	2.67524600
C	2.02623300	0.32942000	2.46455800
C	-0.20939800	0.88804900	4.04721900
H	-1.35859500	0.72664700	2.24028900
C	2.17682800	0.53715100	3.83976400
H	2.90024600	0.09451600	1.86172500
C	1.06078200	0.81808800	4.63123500
H	-1.08419500	1.09525100	4.65816600
H	3.16542300	0.46744900	4.28631900
H	1.17642400	0.97305300	5.70144800
C	-0.88602900	-0.90486100	-0.19159700
C	-0.70258600	-2.28617800	-0.38961100
C	-2.18435600	-0.37614400	-0.13858400
C	-1.81677700	-3.11815700	-0.52007900
H	0.29976700	-2.70695800	-0.43100400
C	-3.29249900	-1.21409900	-0.27453000
H	-2.35869800	0.68553900	0.00768500
C	-3.10963300	-2.58585700	-0.46312700
H	-1.67361000	-4.18631600	-0.66743300
H	-3.98738800	-3.21873400	-0.55464000
S	-4.96643900	-0.47379500	-0.24286900
O	-5.09899700	0.13671700	-1.59648300
O	-5.87085900	-1.62872100	0.01036000
O	-4.88392400	0.51735100	0.86817100
C	4.90633200	0.32252100	-2.23905100
H	5.46513800	0.34388900	-3.18749000
H	4.27283700	1.21789700	-2.21238900
H	5.62964300	0.40411400	-1.41980300

Filename: TS_CuCO2EtPPh3SO3_2
Sum of electronic and zero-point Energies = -57809.6258

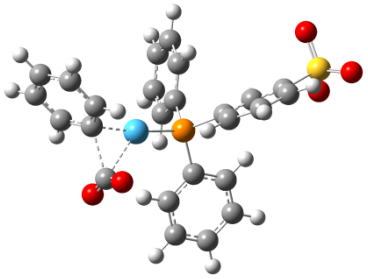


TS $[(PhCH_2CO_2)Cu(PPh_2C_6H_4SO_3)]^-$ → $[(PhCH_2)Cu(PPh_2C_6H_4SO_3)]^-$
(-237 cm^{-1})

Cu	-2.22163800	0.22163500	-0.62343400
O	-4.15048400	2.02498700	-2.23283300
C	-4.03602400	1.37892700	-1.21634900
O	-4.17068800	1.47235100	0.00575400
C	-3.84724400	-0.55352900	-1.79390300
H	-4.91959600	-0.43589300	-1.95874200
H	-3.35556600	-0.59186300	-2.76947800
P	-0.18283200	0.66253400	0.13846700
C	0.10180300	0.00916400	1.83721400
C	0.90510000	0.67404800	2.77609800
C	-0.49293200	-1.21393600	2.18831300
C	1.11858900	0.11854200	4.04031000
H	1.37073600	1.62192700	2.52423000
C	-0.27490200	-1.76780700	3.45114200
H	-1.12510400	-1.73912900	1.47693400
C	0.53163300	-1.10309000	4.37952300
H	1.75459500	0.63724900	4.75295900
H	-0.73605200	-2.71841500	3.70638800
H	0.70525200	-1.53710800	5.36114600
C	0.12382100	2.47587900	0.26934600
C	1.39409000	3.03750600	0.06339500
C	-0.95827600	3.31441300	0.58785200
C	1.57932600	4.41770800	0.18723300
H	2.23845300	2.40608200	-0.19781200
C	-0.76676200	4.69237500	0.71321800
H	-1.95350800	2.89672900	0.72220600
C	0.50200200	5.24611200	0.51460100
H	2.56781300	4.84012200	0.02532000
H	-1.61311600	5.33118100	0.95283700
H	0.64844400	6.31994400	0.60523000
C	1.17604600	-0.00098400	-0.89508000
C	0.95777300	-0.12957700	-2.27942100
C	2.43037100	-0.32381700	-0.35856100
C	1.99394400	-0.56291100	-3.10804000
H	-0.01274700	0.11802700	-2.70456600
C	3.46593700	-0.75075800	-1.19505900
H	2.62832500	-0.23688000	0.70527100
C	3.24834800	-0.87109700	-2.56867600
H	1.82342600	-0.65712600	-4.17845500
H	4.07232600	-1.19410400	-3.19789000
S	5.09670500	-1.14879700	-0.46204300
O	4.88112900	-2.47353400	0.18424900
O	6.02066700	-1.16866200	-1.62987200
O	5.32148800	-0.02853000	0.49641600
C	-3.58073100	-1.74315900	-0.92527600
C	-4.34733600	-1.97601900	0.24079500
C	-2.56344500	-2.67666000	-1.23466700
C	-4.11641800	-3.09375800	1.04313900
H	-5.12095100	-1.26190900	0.51112300
C	-2.33458600	-3.79380000	-0.42886600
H	-1.95789000	-2.52580000	-2.12579300
C	-3.11122200	-4.01167900	0.71440700
H	-4.72368300	-3.24824200	1.93247300
H	-1.54547000	-4.49292200	-0.69515400
H	-2.93333200	-4.88198100	1.34119000

Filename: TS_CuCO2CH2PhPPh3SO3_5
Sum of electronic and zero-point Energies = -63025.9912

Figure S40: Cartesian coordinates and transition state energies (eV) for decarboxylation from $[(RCO_2)Cu(P^*)]^-$ (R = Me, Et, Ph, CH_2Ph).

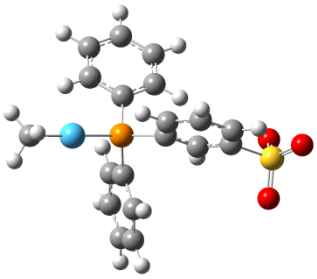


TS [($PhCO_2$)Cu($PPh_2C_6H_4SO_3$)]$^-$ → [(Ph)Cu($PPh_2C_6H_4SO_3$)]$^-$
(-237 cm^{-1})

Cu	-2.13103300	-0.18663100	-0.29635500
O	-3.71312200	0.15037700	-2.81837300
C	-3.91276500	0.63559000	-1.73058300
O	-4.19244800	1.65015500	-1.12778400
P	-0.03983300	0.49638400	0.09845500
C	0.34636900	0.35220800	1.89679200
C	0.21626400	1.45235200	2.75793200
C	0.68258300	-0.90121700	2.43555000
C	0.42543800	1.30252800	4.13202100
H	-0.03786400	2.42995400	2.35847500
C	0.89825900	-1.04544200	3.80694800
H	0.80449900	-1.76190700	1.78389600
C	0.76833400	0.05521700	4.65949600
H	0.33013900	2.16593300	4.78607700
H	1.18282600	-2.01617800	4.20394000
H	0.94361100	-0.05771800	5.72649700
C	0.24258700	2.27213400	-0.30703500
C	1.53712900	2.81853200	-0.35446000
C	-0.86350000	3.09443100	-0.57531200
C	1.71659300	4.16960900	-0.65600100
H	2.40743200	2.19599000	-0.16890400
C	-0.67786000	4.44837000	-0.87508000
H	-1.87058200	2.68451200	-0.56702400
C	0.61017400	4.98708600	-0.91429000
H	2.72291700	4.57867400	-0.69444800
H	-1.54263100	5.07193300	-1.08728800
H	0.75491100	6.03796500	-1.15416400
C	1.25948600	-0.45458300	-0.76788900
C	0.93157100	-1.08634700	-1.98170500
C	2.57394700	-0.52466600	-0.28269900
C	1.91964200	-1.76589600	-2.69748200
H	-0.08491300	-1.04041300	-2.36646800
C	3.55610500	-1.20686900	-1.00305700
H	2.85813500	-0.05417700	0.65370000
C	3.23033600	-1.82654800	-2.21153500
H	1.66434700	-2.24960600	-3.63776000
H	4.01434400	-2.34169200	-2.75859500
S	5.25055900	-1.29919100	-0.31588800
O	5.13809100	-2.34142500	0.74375800
O	6.09445700	-1.68407900	-1.48038200
O	5.48545400	0.07842900	0.20437200
C	-3.97343700	-0.92183700	-0.37954800
C	-4.08877500	-2.20410600	-0.95781400
C	-4.74524300	-0.65317500	0.77089200
C	-4.89699500	-3.19078700	-0.38609600
H	-3.55803300	-2.41594500	-1.88369400
C	-5.55852200	-1.63340000	1.34876500
H	-4.72628000	0.34768000	1.19761200
C	-5.63027700	-2.90661300	0.77249200
H	-4.96662500	-4.17459200	-0.84626600
H	-6.14360500	-1.40440800	2.23753300
H	-6.26825100	-3.66950500	1.21402400

Filename: TS_CuCO2PPh3SO3_2
Sum of electronic and zero-point Energies = -61957.1227

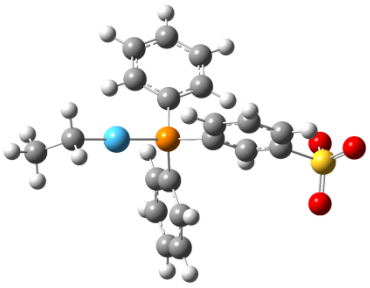
Figure S40 (cont'd): Cartesian coordinates and transition state energies (eV) for decarboxylation from [(RCO_2)Cu(P*)]$^-$ (R = Me, Et, Ph, CH_2Ph).



[(Me)Cu($PPh_2C_6H_4SO_3$)]$^-$

Cu	2.88870400	0.15517200	1.80565000
P	1.20068500	0.01033600	0.29755200
C	1.49565700	-1.28076800	-0.99379000
C	2.81045700	-1.73419600	-1.19071300
C	0.46344200	-1.81997100	-1.78022100
C	3.09336000	-2.69688600	-2.16492300
H	3.61331900	-1.33864600	-0.57240500
C	0.74751700	-2.78474500	-2.74985500
H	-0.56431300	-1.50026900	-1.63683600
C	2.06141400	-3.22325200	-2.94658900
H	4.11634500	-3.03877300	-2.30415700
H	-0.06304500	-3.19375600	-3.34764100
H	2.27744700	-3.97663700	-3.70074100
C	0.98354000	1.57028300	-0.66818600
C	1.52744400	1.72936600	-1.95163800
C	0.34278600	2.66458300	-0.06202100
C	1.42736100	2.95491500	-2.61746700
H	2.02146400	0.89511800	-2.44111400
C	0.23710700	3.88435200	-0.73171200
H	-0.09798000	2.55896500	0.92555000
C	0.78097100	4.03457600	-2.01132000
H	1.84546600	3.05829800	-3.61610900
H	-0.28358000	4.71208700	-0.25726200
H	0.69173300	4.98336000	-2.53481000
C	-0.45800400	-0.35222300	0.98813800
C	-1.64212300	-0.06185100	0.29389200
C	-0.52896300	-0.99458500	2.23840800
C	-2.88097600	-0.43215900	0.82228300
H	-1.62060200	0.44849600	-0.66457300
C	-1.77113500	-1.35299900	2.76630900
H	0.38303000	-1.21003600	2.79056600
C	-2.94658300	-1.07864800	2.05819000
H	-1.82183200	-1.84936600	3.73322200
H	-3.92165900	-1.36204600	2.44312800
S	-4.39713100	-0.05752600	-0.13268000
O	-4.07074000	-0.56003000	-1.49901900
O	-4.51743400	1.42508100	-0.04124200
O	-5.46868400	-0.81456600	0.57246000
C	4.34295400	0.27165500	3.07063600
H	4.01048900	0.00570000	4.08603400
H	5.16809500	-0.40760300	2.80518000
H	4.75453700	1.29192100	3.11358300

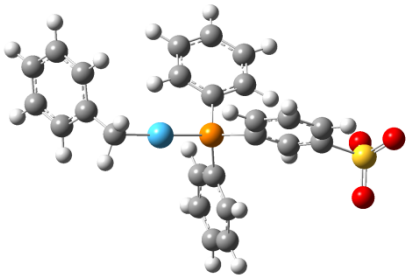
Filename: CuMePPh3SO3_4
Sum of electronic and zero-point Energies = -51609.9021



[(Et)Cu($PPh_2C_6H_4SO_3$)]$^-$

Cu	2.83502300	-1.23490800	-0.76536600
P	1.00539400	-0.05382300	-0.11373100
C	1.12730600	1.74757200	-0.51526200
C	2.39788900	2.28350900	-0.78236800
C	0.00659000	2.59412900	-0.56214700
C	2.55036700	3.64232100	-1.07626300
H	3.26892800	1.63194600	-0.76985900
C	0.16050100	3.95028600	-0.85993000
H	-0.98919800	2.20256500	-0.37720300
C	1.43096900	4.47798400	-1.11471000
H	3.54069400	4.04172300	-1.28239400
H	-0.71707800	4.59080600	-0.89510500
H	1.54563600	5.53391000	-1.34894600
C	0.75938900	-0.09092400	1.71658100
C	1.19580500	0.95504500	2.54372700
C	0.21367200	-1.24257800	2.30941500
C	1.08266700	0.85442100	3.93376900
H	1.61537200	1.85645300	2.10659300
C	0.09462100	-1.33744500	3.69665900
H	-0.14355900	-2.05840100	1.68693200
C	0.53056500	-0.28988300	4.51411800
H	1.41634500	1.67864300	4.55994500
H	-0.35280800	-2.22525300	4.13592400
H	0.43066000	-0.36209200	5.59439000
C	-0.59319300	-0.60907300	-0.81773100
C	-1.82591500	-0.30024800	-0.22323900
C	-0.56969400	-1.32494900	-2.02929600
C	-3.02219400	-0.67322000	-0.84032700
H	-1.87628300	0.23611700	0.71978000
C	-1.76888000	-1.70382100	-2.63639500
H	0.38166700	-1.58171600	-2.48978700
C	-2.99487000	-1.37433000	-2.04758900
H	-1.74643900	-2.25709000	-3.57301800
H	-3.93907500	-1.64596000	-2.51015000
S	-4.60671100	-0.22581500	-0.04020700
O	-4.42963800	1.22072600	0.27911900
O	-4.66259900	-1.11185300	1.15678900
O	-5.63423900	-0.51573100	-1.07878400
C	4.40291100	-2.23362600	-1.33600100
H	4.11587300	-3.29617700	-1.41114600
H	4.65213000	-1.92458700	-2.36541700
C	5.66008300	-2.11022000	-0.45026900
H	6.00950500	-1.07037200	-0.38051800
H	5.46764800	-2.44580800	0.57810600
H	6.51103400	-2.70681400	-0.82667000

Filename: CuEtPPh3SO3_2
Sum of electronic and zero-point Energies = - -52678.7408

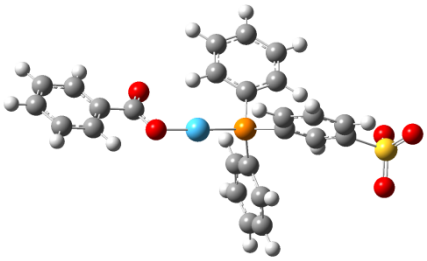


[($PhCH_2$)Cu($PPh_2C_6H_4SO_3$)]$^-$

Cu	-1.96073400	-0.35431500	-1.28895600
P	-0.09458300	0.12973900	-0.11183600
C	-0.34028400	-0.10401700	1.70503200
C	-1.65295700	-0.20994800	2.19354300
C	0.73378400	-0.17563500	2.60853300
C	-1.89060300	-0.37129800	3.56243500
H	-2.49346700	-0.17520000	1.50391900
C	0.49374000	-0.34088100	3.97434500
H	1.75838400	-0.11410500	2.25467600
C	-0.81723500	-0.43629100	4.45443700
H	-2.91272200	-0.45348700	3.92381700
H	1.33521200	-0.39853600	4.66006300
H	-0.99927200	-0.56762500	5.51862900
C	0.38738200	1.90418100	-0.28263400
C	-0.06871900	2.87071400	0.62722200
C	1.13166200	2.31916200	-1.39988500
C	0.22093400	4.22356100	0.42806400
H	-0.64274200	2.56988400	1.49906500
C	1.42555000	3.67034200	-1.59229100
H	1.50743400	1.58648400	-2.10845500
C	0.96992500	4.62709300	-0.68029000
H	-0.13162900	4.95905800	1.14733000
H	2.02449300	3.97036800	-2.44815800
H	1.20589700	5.67812700	-0.82789500
C	1.40592600	-0.82388800	-0.55059700
C	2.69708200	-0.38421500	-0.21989300
C	1.24214800	-2.06288100	-1.19688000
C	3.80967700	-1.17680700	-0.50772400
H	2.86039300	0.57232200	0.26737800
C	2.35953900	-2.84975200	-1.48614500
H	0.24673900	-2.40754600	-1.46795300
C	3.64182700	-2.41154700	-1.13905700
H	2.22801300	-3.80858800	-1.98319700
H	4.52133000	-3.01558600	-1.34151000
S	5.47592600	-0.55639200	-0.07167600
O	5.27344400	0.05411500	1.27388900
O	5.77638000	0.42730600	-1.15041600
O	6.33197300	-1.77474300	-0.08561700
C	-3.63571200	-0.73775300	-2.22903500
H	-3.72671000	-0.00420400	-3.04172400
H	-3.54307500	-1.73490900	-2.68046300
C	-4.80018100	-0.66787200	-1.30431100
C	-5.26055300	-1.80300000	-0.59857100
C	-5.49332900	0.54210600	-1.07101200
C	-6.33733100	-1.73329500	0.28733200
H	-4.75511300	-2.75533900	-0.75272600
C	-6.57047000	0.61549700	-0.18619000
H	-5.17000600	1.43937000	-1.59687600
C	-7.00524200	-0.52206500	0.50517400
H	-6.65996500	-2.63305700	0.80900900
H	-7.07659200	1.56809700	-0.03719200
H	-7.84512100	-0.46668300	1.19387900

Filename: CuCH2PhPPh3SO3_3
Sum of electronic and zero-point Energies = -57895.3106

Figure S41: Cartesian coordinates and energies (eV) for [(R)Cu($PPh_2C_6H_4SO_3$)]$^-$, R = Me, Et, Ph and CH_2Ph.

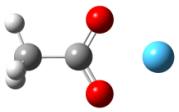


[(Ph)Cu(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

Cu	2.44046800	-0.37156200	0.01603500
P	0.31392200	0.39093600	-0.02470800
C	0.07769500	1.74591600	-1.25949100
C	1.21479100	2.42564400	-1.72674400
C	-1.18803700	2.12025200	-1.74165200
C	1.09050600	3.47029000	-2.64812300
H	2.20119700	2.13116700	-1.37490000
C	-1.30903700	3.16101400	-2.66556900
H	-2.08190200	1.60052600	-1.41035100
C	-0.17248800	3.83948700	-3.11855800
H	1.98041800	3.98573700	-3.00149400
H	-2.29497000	3.43597700	-3.03142100
H	-0.27153800	4.64725900	-3.84003600
C	-0.18364300	1.14690400	1.58500600
C	-0.12127800	2.53190300	1.79994400
C	-0.54125100	0.30760900	2.65397700
C	-0.41635100	3.06735100	3.05737200
H	0.14684600	3.19840500	0.98535400
C	-0.84201800	0.84540500	3.90620900
H	-0.61086000	-0.76637200	2.50439100
C	-0.77864900	2.22703100	4.11270600
H	-0.37327500	4.14384900	3.20526400
H	-1.14015700	0.18366200	4.71517000
H	-1.02035700	2.64505100	5.08682100
C	-0.97662300	-0.85577700	-0.38686400
C	-2.32596100	-0.64892700	-0.06279300
C	-0.59852800	-2.03135600	-1.06166300
C	-3.29330800	-1.58564100	-0.43233400
H	-2.64652700	0.23996600	0.47252200
C	-1.56935500	-2.96954200	-1.41910700
H	0.44714400	-2.20783300	-1.30340500
C	-2.91599000	-2.74623200	-1.11132200
H	-1.27360700	-3.87728700	-1.94076700
H	-3.68840500	-3.45488800	-1.39502100
S	-5.04423200	-1.26086000	-0.00797100
O	-5.23241100	0.16215500	-0.41438400
O	-5.09955100	-1.48743500	1.46379000
O	-5.80494300	-2.25011600	-0.82044600
C	4.26963200	-0.96521400	0.03077300
C	5.03929000	-1.01433000	1.21700900
C	4.93812500	-1.37749500	-1.14605800
C	6.37360400	-1.44174100	1.23428100
H	4.58902100	-0.71201900	2.16231300
C	6.27174400	-1.80776100	-1.14629400
H	4.40688400	-1.36675800	-2.09782200
C	6.99833900	-1.84174800	0.04838200
H	6.92553600	-1.46350000	2.17359100
H	6.74334200	-2.11730000	-2.07860700
H	8.03452200	-2.17571100	0.05533700

Filename: CuPhPPh3SO3_2
Sum of electronic and zero-point Energies = -56826.1223

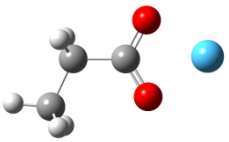
Figure S41 (cont'd): Cartesian coordinates and energies (eV) for [(R)Cu(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$, R = Me, Et, Ph and CH$_2$Ph.



$[Cu(O_2CMe)]^-$

Cu	1.30636500	-0.00250600	0.00167400
O	-0.44155700	1.11650400	-0.00402300
O	-0.44521900	-1.10518700	-0.00418600
C	-1.06975100	0.00762900	-0.00634600
C	-2.58401000	-0.00059400	0.00224500
H	-2.98077900	1.00581800	-0.14103000
H	-2.95445800	-0.66978600	-0.78037300
H	-2.93256500	-0.39609500	0.96312600

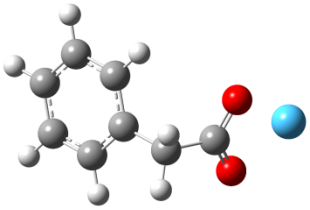
Filename: CuCO2Me
Sum of electronic and zero-point Energies = -11586.8469



$[Cu(O_2CEt)]^-$

O	0.20974700	1.25460000	0.00001900
O	-0.23668600	-0.92072200	-0.00002500
C	-0.62887200	0.28989200	-0.00000600
C	-2.11282500	0.62523700	-0.00002800
H	-2.29190900	1.26616700	0.87302500
H	-2.29189400	1.26606800	-0.87315800
C	-3.05040400	-0.58305700	0.00002800
H	-4.09519000	-0.25011600	-0.00001500
H	-2.88919100	-1.21011500	-0.88261400
H	-2.88923200	-1.21000300	0.88275700
Cu	1.70432900	-0.15605000	0.00000300

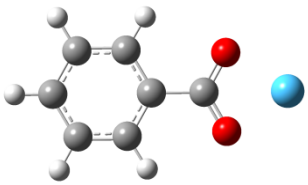
Filename: CuCO2Et
Sum of electronic and zero-point Energies = -12655.8755



$[Cu(O_2CCH_2Ph)]^-$

O	-1.52145300	1.20881300	-0.21853100
O	-1.45679300	-0.72670400	0.87187400
C	-0.97205800	0.42573400	0.62040900
C	0.31107000	0.85705600	1.32642700
H	0.32357200	1.94834400	1.38518200
H	0.29014500	0.44821800	2.34171100
C	1.54294800	0.35825400	0.58731000
C	1.93389400	-0.98638400	0.67774800
C	2.30320100	1.23086200	-0.20288100
C	3.06154800	-1.44640400	-0.00620200
H	1.34490100	-1.67366000	1.28011600
C	3.43343100	0.77285700	-0.88726700
H	2.00753800	2.27435300	-0.28430500
C	3.81612900	-0.56764900	-0.79089900
H	3.35226500	-2.49098500	0.07508500
H	4.01346000	1.46422000	-1.49366900
H	4.69544100	-0.92508700	-1.32090500
Cu	-2.92352800	-0.30235300	-0.52268400

Filename: CuCO2CH2Ph
Sum of electronic and zero-point Energies = - -17872.0062

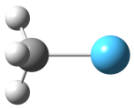


$[Cu(O_2CPh)]^-$

O	-1.08950800	-1.11100300	0.00007300
O	-1.08945300	1.11110200	0.00003700
C	-0.45795000	0.00004100	0.00004400
C	1.03553500	0.00001100	0.00002400
C	1.73896700	1.21410100	0.00001600
C	1.73893100	-1.21410100	0.00000500
C	3.13460800	1.21206200	-0.00001100
H	1.18122600	2.14483800	0.00003600
C	3.13457300	-1.21210400	-0.00002600
H	1.18116500	-2.14482300	0.00001100
C	3.83388200	-0.00003200	-0.00003400
H	3.67711300	2.15401500	-0.00001200
H	3.67704900	-2.15407300	-0.00004400
H	4.92116600	-0.00004700	-0.00005600
Cu	-2.83301100	-0.00001900	-0.00003200

Filename: CuCO2Ph
Sum of electronic and zero-point Energies = -16803.0959

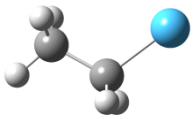
Figure S42: Cartesian coordinates and energies (eV) for $[Cu(O_2CR)]^-$, R = Me, Et, Ph and CH_2Ph.



[Cu(Me)]⁻

C	1.42044000	0.00000100	-0.00002100
H	1.76344600	-0.89054200	-0.53602600
H	1.76325200	0.90956700	-0.50316600
H	1.76363500	-0.01894800	1.03916700
Cu	-0.47630900	-0.00000300	0.00000500

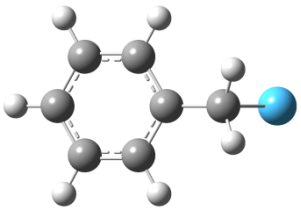
Filename: CuMe
Sum of electronic and zero-point Energies = -6455.0007



[Cu(Et)]⁻

C	0.86796500	0.66177400	0.00000100
H	0.89756700	1.30353000	-0.88913900
H	0.89759000	1.30355300	0.88912300
C	1.99973700	-0.36779300	0.00000000
H	2.97985600	0.13690700	-0.00002700
H	1.96914700	-1.01477500	0.88400100
H	1.96911400	-1.01480700	-0.88397500
Cu	-0.89377500	-0.08545800	0.00000000

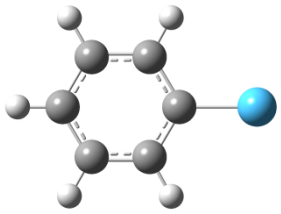
Filename: CuEt
Sum of electronic and zero-point Energies = -6455.0007



[Cu(CH$_2$Ph)]⁻

C	0.96957800	-0.00001900	1.04417600
H	1.20764600	-0.89513700	1.62788500
H	1.20765000	0.89507000	1.62792700
C	-0.42309200	-0.00000700	0.52082500
C	-1.11047400	-1.20552800	0.27546500
C	-1.11046100	1.20552300	0.27548100
C	-2.42401100	-1.20691200	-0.19555200
H	-0.60317200	-2.15100600	0.45809800
C	-2.42399900	1.20692100	-0.19553700
H	-0.60315500	2.15099600	0.45812500
C	-3.09006700	0.00000900	-0.43635700
H	-2.93090700	-2.15279300	-0.37242500
H	-2.93088700	2.15280700	-0.37240500
H	-4.11328200	0.00001800	-0.80294800
Cu	2.29107800	0.00000400	-0.35707800

Filename: CuCH2Ph
Sum of electronic and zero-point Energies = -12740.2902

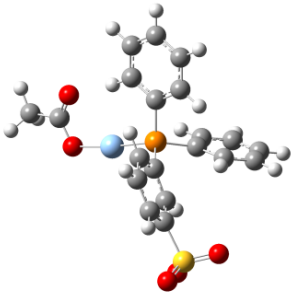


[Cu(Ph)]⁻

C	0.08627900	0.00000300	0.00017000
C	-0.63132300	-1.20914200	0.00011300
C	-0.63132400	1.20914500	0.00011500
C	-2.03216700	-1.20779300	-0.00002700
H	-0.10840900	-2.16191300	0.00017900
C	-2.03216800	1.20779100	-0.00003300
H	-0.10841300	2.16191600	0.00020400
C	-2.73580300	-0.00000100	-0.00011300
H	-2.57086600	-2.15318500	-0.00004100
H	-2.57086700	2.15318200	-0.00005300
H	-3.82321300	-0.00000100	-0.00021400
Cu	1.96692400	0.00000000	-0.00004900

Filename: CuPh
Sum of electronic and zero-point Energies = -11671.0131

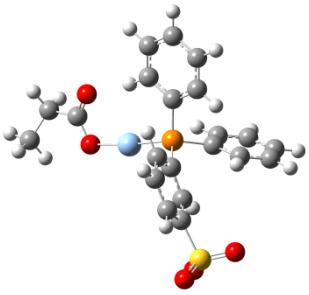
Figure S43: Cartesian coordinates and energies (eV) for [Cu(R)]⁻, R = Me, Et, Ph and CH_2Ph.



$[(CH_3CO_2)Ag(PPh_2C_6H_4SO_3)]^-$

P	0.37335900	0.47994200	0.01096600
C	1.21944500	1.78593200	-0.98539500
C	2.54186600	1.58587000	-1.41179900
C	0.56592900	2.98743300	-1.31091000
C	3.19634700	2.57427600	-2.15727300
H	3.07292200	0.66828300	-1.16445900
C	1.22221700	3.96978100	-2.05262100
H	-0.45772700	3.15564700	-0.98787600
C	2.54053600	3.76407600	-2.47817600
H	4.22031100	2.40507300	-2.48031300
H	0.70527800	4.89422300	-2.29894600
H	3.05116700	4.53088300	-3.05631400
C	-0.19316200	1.37323500	1.52375600
C	-1.43455700	2.02369100	1.60857700
C	0.68028300	1.42443700	2.62256400
C	-1.78973900	2.71474200	2.77013000
H	-2.14234500	1.96992700	0.78745600
C	0.32819800	2.12559600	3.77775100
H	1.63650800	0.90760000	2.57767000
C	-0.90947200	2.77150300	3.85396700
H	-2.76441400	3.19187300	2.82811300
H	1.01397200	2.15264800	4.62104300
H	-1.19296300	3.30283400	4.75930400
C	-1.14273600	0.05291200	-0.92837400
C	-2.24087500	-0.50644000	-0.25530600
C	-1.19080000	0.20543100	-2.32510000
C	-3.39573700	-0.85441800	-0.95827500
H	-2.22746300	-0.66966400	0.81875800
C	-2.33509600	-0.18537700	-3.02579700
H	-0.34579300	0.62425600	-2.86374000
C	-3.44141300	-0.70278900	-2.34638300
H	-2.36374400	-0.07343800	-4.10772000
H	-4.34344000	-0.99891300	-2.87344900
S	-4.87835700	-1.39377800	-0.02927500
O	-5.47981400	-0.09739500	0.40209500
O	-4.32949400	-2.21324800	1.08590600
O	-5.68479000	-2.14469800	-1.03030400
O	4.57884400	-1.30304800	-0.52594700
O	3.43101100	-2.76935600	0.73853600
C	4.49202400	-2.36833900	0.11700400
C	5.68682100	-3.31408300	0.21375200
H	6.55297400	-2.89825000	-0.30685500
H	5.93649500	-3.49295900	1.26600900
H	5.42492600	-4.28426500	-0.22466100
Ag	1.91808800	-1.28994300	0.42840600

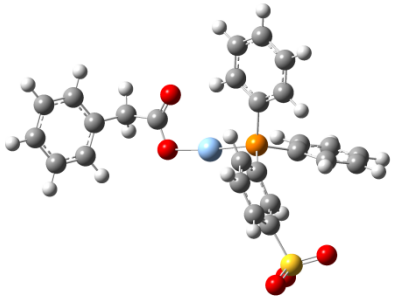
Filename: AgCO2MePPh3SO3_5
Sum of electronic and zero-point Energies = -55372.0571



$[(CH_3CH_2CO_2)Ag(PPh_2C_6H_4SO_3)]^-$

P	0.11993300	0.65390600	0.01685300
C	0.76663300	2.10119600	-0.93242900
C	2.09635600	2.09762700	-1.38238100
C	-0.04690200	3.21643300	-1.19887900
C	2.60002900	3.19406000	-2.09312100
H	2.74930600	1.25046600	-1.17970100
C	0.45944100	4.30699000	-1.90611600
H	-1.07794800	3.23283700	-0.85653400
C	1.78578400	4.29714100	-2.35567500
H	3.63170800	3.17696000	-2.43493900
H	-0.18037900	5.16303800	-2.10687900
H	2.17940200	5.14818600	-2.90682500
C	-0.54235500	1.40159500	1.56922400
C	-1.86141600	1.86632200	1.69307200
C	0.33294400	1.53457500	2.65970400
C	-2.29152300	2.45583900	2.88492400
H	-2.56774500	1.74420600	0.87805700
C	-0.09550100	2.13500800	3.84538700
H	1.35160700	1.16022500	2.58406200
C	-1.41054300	2.59580700	3.96055700
H	-3.32266300	2.78770900	2.97221900
H	0.59330000	2.22720300	4.68157900
H	-1.75130900	3.04718900	4.88923600
C	-1.33639400	0.06057500	-0.92667700
C	-2.33545900	-0.67469400	-0.26854200
C	-1.42742500	0.26493700	-2.31458300
C	-3.44201800	-1.14941300	-0.97496100
H	-2.28226700	-0.88065600	0.79693000
C	-2.51754000	-0.25095100	-3.02080500
H	-0.65739900	0.82007000	-2.84223900
C	-3.53042200	-0.94602300	-2.35439800
H	-2.57868400	-0.09773200	-4.09630000
H	-4.39091700	-1.34197700	-2.88535300
S	-4.82060800	-1.92937200	-0.05666500
O	-5.59052500	-0.74910900	0.43591000
O	-4.14586500	-2.70952000	1.01688200
O	-5.52935300	-2.74354100	-1.08186500
O	4.49988700	-0.52752000	-0.61631800
O	3.59697900	-2.18570200	0.60389200
C	4.57995400	-1.61760600	-0.01193400
C	5.93050900	-2.34042800	0.05668100
H	6.49585600	-2.06830200	-0.84181900
H	6.47581000	-1.90026800	0.90518000
Ag	1.89677000	-0.90352600	0.35113300
C	5.84976600	-3.86082500	0.22557400
H	6.85530100	-4.29783100	0.29119500
H	5.29331800	-4.12432300	1.12999400
H	5.33377100	-4.32575500	-0.62298300

Filename: AgCO2EtPPh3SO3_3
Sum of electronic and zero-point Energies = -56441.0707

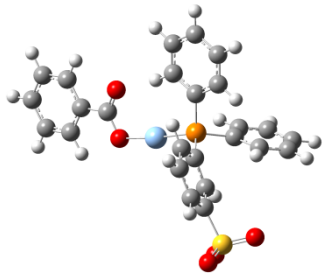


$[(PhCH_2CO_2)Ag(PPh_2C_6H_4SO_3)]^-$

P	0.91262500	0.86272400	0.06977600
C	0.60954500	2.16225700	1.34885600
C	-0.69987500	2.60850300	1.58613800
C	1.67188900	2.73361400	2.07109900
C	-0.94034800	3.61054200	2.53405200
H	-1.53876800	2.18448800	1.03732800
C	1.42806600	3.73196000	3.01436200
H	2.69009900	2.39378100	1.90367600
C	0.11949000	4.17284400	3.24758700
H	-1.96007300	3.94458800	2.70740300
H	2.25824100	4.16397700	3.56803400
H	-0.06924900	4.95066800	3.98396200
C	2.01202700	1.69252100	-1.15792800
C	3.40552200	1.77135700	-1.00191500
C	1.41517800	2.30284200	-2.27286900
C	4.18256500	2.45086200	-1.94299200
H	3.89575800	1.27837300	-0.16843500
C	2.19274700	2.99142600	-3.20690300
H	0.33883400	2.23454800	-2.41505600
C	3.57891600	3.06530300	-3.04385900
H	5.26191300	2.48076700	-1.82045800
H	1.71577500	3.45522300	-4.06680900
H	4.18784600	3.58584500	-3.77904100
C	1.93197600	-0.41351500	0.90234100
C	2.83113900	-1.19373700	0.15859100
C	1.75282800	-0.67884900	2.27199500
C	3.58581100	-2.18808700	0.78467700
H	2.97140300	-1.04195000	-0.90763100
C	2.48376700	-1.70155300	2.88116900
H	1.05048400	-0.09471700	2.85999900
C	3.40824200	-2.44867500	2.14515600
H	2.33583900	-1.90753700	3.93922300
H	3.99371300	-3.23914900	2.60504600
S	4.88334700	-3.05787400	-0.17058100
O	6.02636800	-2.09943300	-0.11403600
O	4.28838200	-3.21891700	-1.52595900
O	5.10241000	-4.32452700	0.58013300
O	-3.67963500	1.40660800	-0.25846800
O	-3.13495900	-0.36551100	-1.53907600
C	-3.97465700	0.46760700	-1.02031100
C	-5.44793800	0.22260600	-1.40176900
H	-5.99728400	1.15733100	-1.25865500
H	-5.48397400	-0.04798600	-2.46331200
Ag	-1.18345600	0.15137300	-0.82194400
C	-6.07814400	-0.87977100	-0.57187700
C	-5.77148400	-2.22875500	-0.81474300
C	-6.97032000	-0.57513800	0.46643900
C	-6.34409800	-3.24210000	-0.04283100
H	-5.06487800	-2.47600900	-1.60264600
C	-7.54583400	-1.58746500	1.24158600
H	-7.20984400	0.46590200	0.67265700
C	-7.23574900	-2.92640700	0.98873600
H	-6.09030900	-4.28044000	-0.24436100
H	-8.23364000	-1.32794200	2.04360200
H	-7.68047000	-3.71607800	1.59003600

Filename: AgCO2CH2PhPPh3SO3_3
Sum of electronic and zero-point Energies = -61657.2555

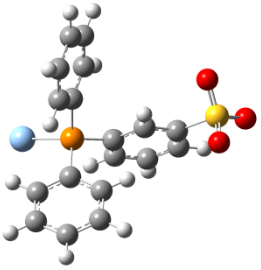
Figure S44: Cartesian coordinates and energies (eV) for $[(RCO_2)Ag(PPh_2C_6H_4SO_3)]^-$, R = Me, Et, Ph and CH_2Ph.



$[(PhCO_2)Ag(PPh_2C_6H_4SO_3)]^-$

P	-0.72070700	0.79300000	0.03783400
C	-0.37004500	2.38397000	-0.83264600
C	0.93469000	2.66463500	-1.26728700
C	-1.38632400	3.33075900	-1.05039900
C	1.21414800	3.87292900	-1.91727300
H	1.74067000	1.95280800	-1.09871400
C	-1.10355300	4.53347900	-1.69803400
H	-2.40052100	3.12771100	-0.71738700
C	0.19909300	4.80651900	-2.13377300
H	2.22929400	4.07622700	-2.24836900
H	-1.89866800	5.25680200	-1.86235600
H	0.41826600	5.74478600	-2.63824600
C	-1.49479700	1.31871900	1.62880300
C	-2.87837800	1.49912500	1.78407700
C	-0.64603800	1.57787400	2.71769400
C	-3.39894600	1.93300500	3.00638000
H	-3.55886800	1.27365200	0.96918800
C	-1.16737500	2.02359800	3.93392600
H	0.42626700	1.42444700	2.61684400
C	-2.54665300	2.20022300	4.08095200
H	-4.47440300	2.04300100	3.11706900
H	-0.49748900	2.21660300	4.76824700
H	-2.95615200	2.52944000	5.03290100
C	-2.04576900	-0.02041600	-0.93358200
C	-2.86837300	-0.97419700	-0.31325600
C	-2.19991600	0.23946400	-2.30675500
C	-3.87281100	-1.61768300	-1.03866100
H	-2.75643200	-1.22422100	0.73819200
C	-3.17944000	-0.44163100	-3.03451800
H	-1.56374500	0.96411300	-2.80641700
C	-4.02426500	-1.35883200	-2.40307600
H	-3.28871900	-0.24380300	-4.09884800
H	-4.80018300	-1.88594000	-2.95015400
S	-5.05190100	-2.70450000	-0.15527200
O	-6.00100500	-1.72541300	0.45211000
O	-4.20598900	-3.42827000	0.83311700
O	-5.64182000	-3.55289900	-1.22672300
O	3.85783900	0.53058700	-0.55360900
O	3.22217000	-1.37041600	0.47088800
C	4.10594400	-0.58269700	-0.04640000
Ag	1.31656600	-0.42069000	0.28897400
C	5.53181300	-1.08795600	-0.01078900
C	5.83999300	-2.34584300	0.52718500
C	6.56445500	-0.28965700	-0.52288800
C	7.16181300	-2.79843600	0.55188800
H	5.03239100	-2.95522500	0.91966100
C	7.88626300	-0.74033900	-0.49704700
H	6.30814800	0.68073100	-0.93679600
C	8.18834500	-1.99679700	0.04058900
H	7.39133000	-3.77647600	0.96924800
H	8.68091700	-0.11355000	-0.89625300
H	9.21751100	-2.34924900	0.06032400

Filename: AgCO2PhPPh3SO3_2
Sum of electronic and zero-point Energies = -60588.3431

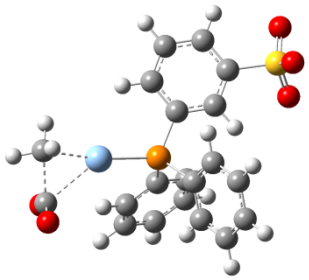


$[Ag(PPh_2C_6H_4SO_3)]^-$

P	-1.06742700	-0.01083100	-0.22183300
C	-1.52556000	-1.08227600	1.19114700
C	-2.87314200	-1.36835100	1.46150700
C	-0.52187000	-1.60324100	2.02669300
C	-3.21860600	-2.15584900	2.56193200
H	-3.65725000	-0.97994200	0.81375400
C	-0.87437800	-2.39124300	3.12472300
H	0.52714700	-1.40412800	1.82826400
C	-2.21815400	-2.66750000	3.39415100
H	-4.26392400	-2.37359800	2.76353000
H	-0.09218000	-2.79020500	3.76419200
H	-2.48521300	-3.28552400	4.24707800
C	-0.91523800	1.69813400	0.40536700
C	-1.53447000	2.08509800	1.60506900
C	-0.19995100	2.64609400	-0.34842400
C	-1.43037900	3.40576700	2.04778400
H	-2.07742900	1.35974200	2.20325300
C	-0.09469700	3.96055100	0.10511900
H	0.30456500	2.35517300	-1.26551700
C	-0.71124700	4.34289300	1.30117300
H	-1.89841000	3.69578300	2.98442100
H	0.48569000	4.67893700	-0.46631600
H	-0.61961300	5.36576100	1.65571200
C	0.54247400	-0.53029400	-0.86158400
C	1.71034200	-0.08756200	-0.22328300
C	0.62366500	-1.44732300	-1.92784200
C	2.95306800	-0.57481300	-0.63075700
H	1.68083200	0.63004500	0.59114300
C	1.87215100	-1.91304600	-2.33833900
H	-0.27818500	-1.79557500	-2.42897000
C	3.03623900	-1.48200000	-1.68759800
H	1.93962500	-2.61256300	-3.16779500
H	4.01821800	-1.83285800	-1.99148000
S	4.42777300	-0.02779000	0.31139800
O	4.20470200	-0.68743700	1.62825300
O	4.27578600	1.45183600	0.33317000
O	5.56979800	-0.54765600	-0.47934600
Ag	-2.73490600	-0.15208800	-1.96348500

Filename: AgPPh3SO3
Sum of electronic and zero-point Energies = -49150.8208

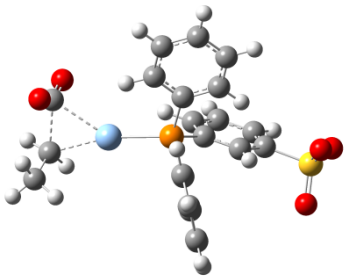
Figure S44 (cont'd): Cartesian coordinates and energies (eV) for $[(RCO_2)Ag(PPh_2C_6H_4SO_3)]^-$, R = Me, Et, Ph and CH_2Ph, and for $[Ag(PPh_2C_6H_4SO_3)]^-$.



TS $[(CH_3CO_2)Ag(PPh_2C_6H_4SO_3)]^- \rightarrow [(CH_3)Ag(PPh_2C_6H_4SO_3)]^-$
(-377 cm^{-1})

O	5.53827500	-0.63236500	1.09954100
C	5.00055100	-0.81120800	0.03030600
O	4.88442900	-0.32940100	-1.08807800
C	4.23156700	-2.66284000	0.11552700
H	3.52533600	-3.21659400	-0.53211100
H	5.21271800	-2.93099700	-0.28714000
H	4.18220000	-3.01870600	1.14803600
P	0.45067300	0.11895600	-0.00665300
Ag	2.49314200	-1.15856600	0.04723100
C	0.56427000	1.49680400	-1.22718400
C	-0.57379300	2.21912200	-1.62743500
C	1.81747000	1.83073300	-1.76587800
C	-0.45342900	3.26420800	-2.54485800
H	-1.55559600	1.96661100	-1.23837200
C	1.93256200	2.88162100	-2.68238000
H	2.70734200	1.27216400	-1.48388700
C	0.79925300	3.59895000	-3.07188600
H	-1.34194800	3.81104300	-2.84964900
H	2.90878200	3.12771100	-3.09223700
H	0.88795100	4.41206200	-3.78862800
C	-1.05241300	-0.83486600	-0.42529700
C	-2.33673900	-0.36681700	-0.10796900
C	-0.91139700	-2.04181300	-1.13382400
C	-3.46751500	-1.08325600	-0.50440100
H	-2.48247500	0.55520000	0.44654700
C	-2.04614400	-2.75360100	-1.52839100
H	0.07946600	-2.41832600	-1.37864000
C	-3.32353800	-2.27546400	-1.21732800
H	-1.93221100	-3.68440900	-2.07975500
H	-4.21861200	-2.80815600	-1.52452000
C	0.10154500	0.93784200	1.60662400
C	-0.55494000	0.22900800	2.62648500
C	0.57158700	2.23412000	1.86824500
C	-0.74861500	0.81371800	3.87921300
H	-0.93969600	-0.76947700	2.43986800
C	0.38155300	2.81303400	3.12573300
H	1.08036400	2.79757900	1.09141700
C	-0.27993500	2.10610800	4.13307400
H	-1.28003600	0.26167500	4.64975100
H	0.74554600	3.82034900	3.31239000
H	-0.43680400	2.56158900	5.10762800
S	-5.12171900	-0.44865100	-0.04224100
O	-6.05275200	-1.16754900	-0.95432400
O	-5.24449300	-0.82126000	1.39543300
O	-5.00595800	1.01744400	-0.28696500

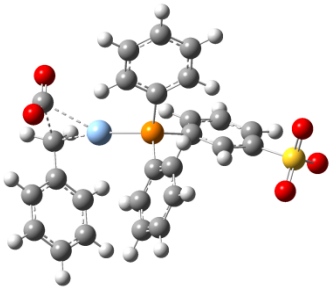
Filename: TS_AgCO2MePPh3SO3_2
Sum of electronic and zero-point Energies = -55370.3488



TS $[(CH_3CH_2CO_2)Ag(PPh_2C_6H_4SO_3)]^- \rightarrow [(CH_3CH_2)Ag(PPh_2C_6H_4SO_3)]^-$
(-334 cm^{-1})

O	-4.24120800	-1.54184000	-2.00850300
C	-4.64714500	-0.96611000	-1.01148200
O	-5.32779500	-0.02271700	-0.66061500
C	-4.31857200	-2.12492200	0.63731900
H	-5.05097700	-2.75443100	0.12319000
H	-3.48858200	-2.83510100	0.82620000
P	-0.31390300	0.26851500	0.02147600
C	0.13515300	0.93350700	1.68134300
C	-0.17245700	2.25486200	2.03960000
C	0.70948400	0.08137400	2.63967700
C	0.09498100	2.71662100	3.33155500
H	-0.61223000	2.92949900	1.31081500
C	0.98218100	0.54844800	3.92630100
H	0.97177600	-0.93972300	2.37726900
C	0.67383200	1.86649400	4.27690300
H	-0.14108500	3.74538900	3.59245900
H	1.45106500	-0.11550600	4.64755000
H	0.89338700	2.23029700	5.27753500
C	-0.35648600	1.74202000	-1.08472300
C	0.82405400	2.38888200	-1.49013200
C	-1.59524600	2.22770400	-1.53189800
C	0.75911000	3.50904800	-2.32071900
H	1.79433500	2.01907500	-1.17190300
C	-1.65605000	3.35207800	-2.36142800
H	-2.51651100	1.72661200	-1.24384300
C	-0.47963100	3.99373300	-2.75575600
H	1.67950500	3.99693600	-2.63089900
H	-2.62232800	3.71349900	-2.70365300
H	-0.52510700	4.86364300	-3.40672400
C	1.10721400	-0.74947000	-0.51258200
C	0.86611000	-1.86023600	-1.34204800
C	2.42483900	-0.41983800	-0.16108700
C	1.93995100	-2.61531900	-1.81780100
H	-0.15159400	-2.12642900	-1.61940200
C	3.49350600	-1.18118500	-0.63825900
H	2.64420400	0.42682000	0.48232400
C	3.25230800	-2.27774900	-1.46851000
H	1.75063800	-3.47046000	-2.46280400
H	4.10102800	-2.84733000	-1.83532100
S	5.19291900	-0.73031900	-0.12759100
O	5.27017300	-1.21532500	1.27961300
O	6.06610400	-1.45928400	-1.08754200
O	5.20795100	0.75442100	-0.26385000
C	-4.89864300	-1.54420800	1.92616100
H	-5.48468000	-2.28958200	2.48688300
H	-4.11940300	-1.16861300	2.60161200
H	-5.56289200	-0.70493100	1.69032000
Ag	-2.42598900	-0.89614300	0.07511200

Filename: TS_AgCO2EtPPh3SO3
Sum of electronic and zero-point Energies = -56439.2744

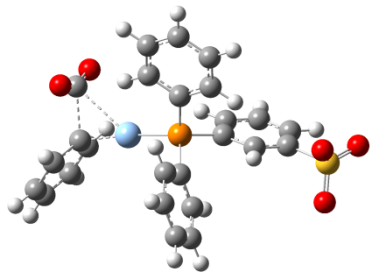


TS $[(PhCH_2CO_2)Ag(PPh_2C_6H_4SO_3)]^- \rightarrow [(PhCH_2)Ag(PPh_2C_6H_4SO_3)]^-$
(-276 cm^{-1})

O	-4.10708900	2.35997300	-2.12141900
C	-4.14571600	1.68029200	-1.11890000
O	-4.35176600	1.73698400	0.08573600
C	-4.09503600	-0.25440100	-1.74511200
H	-5.12551300	0.00177600	-2.00099800
H	-3.56059400	-0.38173100	-2.69295400
P	0.18969000	0.60577200	0.19548000
C	0.37746500	-0.23834400	1.82033200
C	1.24852800	0.23457000	2.81395100
C	-0.36096500	-1.40959100	2.05648700
C	1.38783800	-0.46120600	4.01740500
H	1.82355700	1.14123500	2.65155400
C	-0.21787300	-2.10337400	3.25947800
H	-1.05074700	-1.78384900	1.30362000
C	0.65770000	-1.63112800	4.24155400
H	2.07690000	-0.09237000	4.77264000
H	-0.79346500	-3.00994900	3.42684800
H	0.77219200	-2.17372000	5.17664600
C	0.65708600	2.36083400	0.50816000
C	1.96467200	2.83387800	0.31455200
C	-0.33755900	3.24804300	0.95434600
C	2.27207000	4.17246900	0.57780100
H	2.74472900	2.16841400	-0.04344800
C	-0.02473400	4.58255600	1.21999400
H	-1.36079400	2.90219300	1.08478500
C	1.28137400	5.04693800	1.03236400
H	3.28862600	4.52506300	0.42382500
H	-0.80481200	5.25911700	1.55962300
H	1.52315100	6.08829600	1.23139700
C	1.48899100	-0.07703300	-0.89594400
C	1.25458300	-0.11325300	-2.28270900
C	2.72698700	-0.49967400	-0.39026400
C	2.25984600	-0.55563400	-3.14455600
H	0.29384300	0.20326100	-2.68358100
C	3.73633500	-0.91919600	-1.26048600
H	2.92851800	-0.51322000	0.67653100
C	3.50221000	-0.95174000	-2.63670200
H	2.07292600	-0.59044200	-4.21566700
H	4.29782500	-1.29701600	-3.29021700
S	5.38594100	-1.32176000	-0.57532300
O	5.95961900	0.02735600	-0.29674900
O	5.08296300	-2.11864000	0.64542400
O	6.06325000	-2.07098500	-1.66862500
C	-4.05629900	-1.45833600	-0.86052900
C	-4.88066200	-1.54823800	0.28301500
C	-3.19511300	-2.54681000	-1.12922700
C	-4.84514400	-2.67148100	1.11037500
H	-5.53612600	-0.71560700	0.52304500
C	-3.16066000	-3.66997400	-0.29940300
H	-2.55596800	-2.51317000	-2.01001200
C	-3.98629200	-3.74073400	0.82778100
H	-5.49104500	-2.71115000	1.98513600
H	-2.48986500	-4.49237000	-0.53842600
H	-3.96231900	-4.61497800	1.47384700
Ag	-2.04989400	0.41122700	-0.66678100

Filename: TS_AgCO2CH2PhPPh3SO3_2
Sum of electronic and zero-point Energies = -61655.6445

Figure S45: Cartesian coordinates and transition state energies (eV) for decarboxylation from $[(RCO_2)Ag(P^*)]^-$ (R = Me, Et, Ph, CH_2Ph).

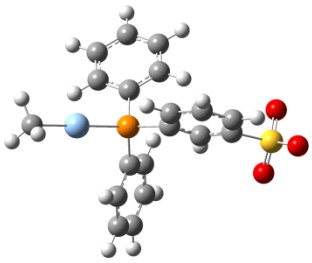


TS [(PhCO$_2$)Ag(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$ → [(Ph)Ag(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$
(-262 cm^{-1})

O	-4.10860500	0.33501700	-2.68506100
C	-4.22921800	0.78073300	-1.57280600
O	-4.44940700	1.75202400	-0.88952400
P	0.23168800	0.50584200	0.12668000
C	0.68972400	0.49037200	1.91251200
C	0.60113500	1.65256300	2.69388700
C	1.04041300	-0.72244800	2.52941900
C	0.86550700	1.60346100	4.06561100
H	0.33645400	2.60031700	2.23413400
C	1.31077800	-0.76609300	3.89799800
H	1.13014000	-1.63048900	1.93974700
C	1.22236900	0.39592500	4.67065100
H	0.80183200	2.51396000	4.65654800
H	1.60562000	-1.70713900	4.35451200
H	1.44050800	0.36113400	5.73511300
C	0.52614400	2.24185900	-0.42115000
C	1.82685000	2.75659500	-0.56287300
C	-0.57410400	3.06769000	-0.70097700
C	2.01714200	4.07868200	-0.96868000
H	2.69324800	2.13123000	-0.36899300
C	-0.37889900	4.39258400	-1.10497100
H	-1.58709800	2.68136800	-0.61474000
C	0.91586400	4.89925700	-1.23812900
H	3.02813000	4.46235400	-1.07884500
H	-1.24085500	5.01794400	-1.32289100
H	1.06894000	5.92712100	-1.55861100
C	1.48057800	-0.52941200	-0.71666300
C	1.09613600	-1.24895100	-1.86267500
C	2.81389900	-0.57967800	-0.28235900
C	2.04630000	-1.99313200	-2.56532800
H	0.06398100	-1.22186000	-2.20519700
C	3.75820500	-1.32690800	-0.98851500
H	3.14255200	-0.04279100	0.60233100
C	3.37590600	-2.03222500	-2.13178700
H	1.74659700	-2.54447300	-3.45384200
H	4.13098900	-2.59631500	-2.67121400
S	5.47902800	-1.38849700	-0.36613700
O	5.40714800	-2.37114600	0.75216700
O	6.27376200	-1.83957400	-1.54115700
O	5.73639700	0.01464900	0.06796000
C	-4.15531900	-0.86153200	-0.27591700
C	-4.33337700	-2.11120000	-0.90812400
C	-4.84101000	-0.64854100	0.93944400
C	-5.12400800	-3.11406500	-0.33872700
H	-3.86981700	-2.28348200	-1.87755400
C	-5.63656700	-1.64404200	1.51691500
H	-4.77379400	0.32623900	1.41900700
C	-5.77421400	-2.88200600	0.87935300
H	-5.24397200	-4.06977300	-0.84576600
H	-6.15690000	-1.45352800	2.45391200
H	-6.39798900	-3.65670300	1.32071800
Ag	-2.06753400	-0.18535100	-0.19557700

Filename: TS_AgCO2PhPPh3SO3
Sum of electronic and zero-point Energies = -60586.8429

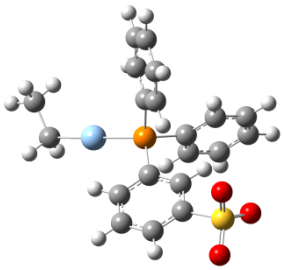
Figure S45 (cont'd): Cartesian coordinates and transition state energies (eV) for decarboxylation from [(RCO$_2$)Ag(P*)]$^-$ (R = Me, Et, Ph, CH$_2$Ph).



[(Me)Ag($PPh_2C_6H_4SO_3$)]$^-$

P	0.95349600	0.00245800	-0.01230500
C	0.95876700	1.38146600	-1.24384400
C	2.15906600	2.09080200	-1.42808000
C	-0.16400000	1.73594500	-2.00763900
C	2.22994600	3.14500700	-2.34035900
H	3.04351600	1.81218700	-0.85908400
C	-0.08883200	2.78872200	-2.92641800
H	-1.10058300	1.19940600	-1.89115300
C	1.10390000	3.49641000	-3.09330300
H	3.16557700	3.68408500	-2.46971300
H	-0.97003500	3.05163800	-3.50606900
H	1.15890500	4.31361500	-3.80883100
C	0.69745100	0.85459000	1.60485000
C	0.09045400	2.11466100	1.71920900
C	1.11771500	0.19323800	2.77098200
C	-0.10534100	2.69396200	2.97585000
H	-0.23853600	2.64452200	0.83011800
C	0.91820900	0.77159700	4.02611900
H	1.60288400	-0.77727200	2.69545200
C	0.30540800	2.02395100	4.13108700
H	-0.59225500	3.66308000	3.04927400
H	1.24245600	0.24411500	4.91991500
H	0.14515400	2.47321200	5.10819500
C	-0.59830700	-0.92251400	-0.32452800
C	-1.85666300	-0.41614500	0.03568400
C	-0.51440100	-2.15458400	-0.99787300
C	-3.02054400	-1.10737800	-0.30776400
H	-1.95524200	0.51597300	0.58393400
C	-1.68124500	-2.85490600	-1.31394200
H	0.45754300	-2.56303400	-1.26552100
C	-2.93344300	-2.32997300	-0.97832700
H	-1.61164900	-3.81317000	-1.82456500
H	-3.85210800	-2.85680700	-1.21887600
S	-4.64644400	-0.33847400	0.03289500
O	-4.77064500	0.66516300	-1.06539900
O	-4.48922200	0.25969200	1.38787900
O	-5.61297200	-1.46830300	-0.05033600
Ag	3.02843000	-1.32606400	-0.07571800
C	4.83179700	-2.43903600	-0.12083700
H	5.53092600	-2.08620300	0.64962800
H	4.63585800	-3.50473000	0.05972400
H	5.32514300	-2.34419500	-1.09778600

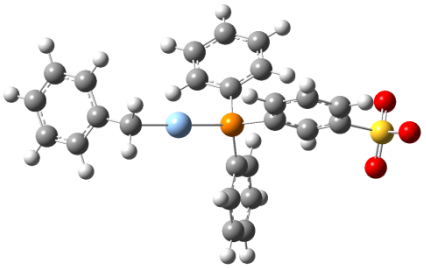
Filename: AgMePPh3SO3_4
Sum of electronic and zero-point Energies = -50239.7027



[(Et)Ag($PPh_2C_6H_4SO_3$)]$^-$

P	0.73915900	0.10333900	0.01476600
C	0.69319000	1.35024600	-1.34934400
C	1.85202100	2.11360100	-1.57834800
C	-0.42632300	1.55176000	-2.17130100
C	1.88419100	3.07203300	-2.59268600
H	2.73485400	1.95264400	-0.96323500
C	-0.38961100	2.50838500	-3.19196100
H	-1.33082400	0.97043800	-2.02125900
C	0.76119500	3.27131300	-3.40363600
H	2.78787500	3.65479900	-2.75536300
H	-1.26802600	2.65350700	-3.81563800
H	0.78637300	4.01348400	-4.19821700
C	0.40354300	1.09641700	1.53390100
C	-0.26706900	2.32891600	1.51172300
C	0.82939000	0.57549300	2.76730100
C	-0.51914200	3.01845800	2.70090000
H	-0.60186400	2.75101800	0.56874600
C	0.57355100	1.26363600	3.95499000
H	1.36313100	-0.37171700	2.79722100
C	-0.10207600	2.48738600	3.92409600
H	-1.05459400	3.96394900	2.66902000
H	0.90297300	0.84392200	4.90239300
H	-0.30606400	3.02194400	4.84869800
C	-0.75192900	-0.93611900	-0.22421100
C	-2.04426000	-0.46787600	0.05996500
C	-0.58468100	-2.22584800	-0.75972000
C	-3.15980600	-1.25828600	-0.22445500
H	-2.20689200	0.50999700	0.50327000
C	-1.70347400	-3.02244300	-1.01648400
H	0.41417300	-2.60335900	-0.96686000
C	-2.98983700	-2.53845100	-0.75806000
H	-1.56938800	-4.02401400	-1.41988800
H	-3.87190400	-3.14100400	-0.95368800
S	-4.83398300	-0.55465300	0.00588100
O	-5.00463200	0.29093200	-1.21259200
O	-4.73168400	0.21978400	1.27406800
O	-5.72851300	-1.74385700	0.06258800
Ag	2.89102300	-1.10682100	0.11637700
C	4.75833200	-2.13696500	0.21997300
H	4.93043000	-2.41093100	1.27182200
H	4.64283800	-3.08675600	-0.32364800
C	5.98398800	-1.37921200	-0.32212000
H	6.91662400	-1.96758900	-0.24167100
H	5.86519000	-1.11623700	-1.38202500
H	6.15483300	-0.43868400	0.21934500

Filename: AgEtPPh3SO3_3
Sum of electronic and zero-point Energies = -51308.5457

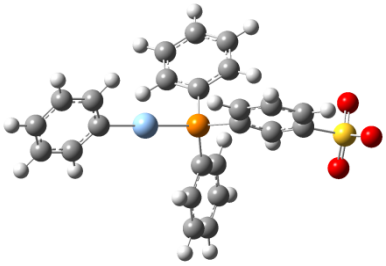


[($PhCH_2$)Ag($PPh_2C_6H_4SO_3$)]$^-$

P	0.12278800	0.11238400	-0.01902000
C	0.09617800	1.01459500	1.59228900
C	-1.10910500	1.61918800	1.99078600
C	1.21701600	1.10920900	2.43241600
C	-1.18770300	2.32068000	3.19559000
H	-1.99227300	1.53502100	1.36113200
C	1.13377200	1.80780300	3.64144600
H	2.15627000	0.64188100	2.15259600
C	-0.06455800	2.41612500	4.02423000
H	-2.12761000	2.78156900	3.48948000
H	2.01192700	1.87343300	4.27872000
H	-0.12574500	2.95679200	4.96585500
C	0.51029400	1.41094200	-1.26992700
C	1.04441600	2.66356800	-0.93425600
C	0.26681700	1.11365100	-2.62158800
C	1.33908600	3.59643500	-1.93306800
H	1.24002600	2.91291000	0.10426300
C	0.56828200	2.04327400	-3.61776600
H	-0.15576400	0.14961100	-2.89587400
C	1.10460300	3.28860800	-3.27501500
H	1.76522700	4.55819400	-1.65900500
H	0.38426200	1.79468300	-4.66002500
H	1.34313700	4.01214100	-4.05063200
C	1.60803100	-0.95829800	0.03968300
C	2.90194700	-0.44076700	-0.12388000
C	1.43742100	-2.32731700	0.31389200
C	4.01659900	-1.26890600	0.02685600
H	3.06530600	0.60463600	-0.36904000
C	2.55554400	-3.15540900	0.43661100
H	0.43709200	-2.74024400	0.42450300
C	3.84407000	-2.62742700	0.30274300
H	2.41992800	-4.21594800	0.63824100
H	4.72631800	-3.25328300	0.39897500
S	5.68943100	-0.52798900	-0.03521000
O	5.80730700	0.12306700	1.30289700
O	5.61930800	0.42947300	-1.17375100
O	6.59841100	-1.68925300	-0.24075800
Ag	-2.00093100	-1.03812700	-0.46257600
C	-3.89407100	-2.00164400	-0.83034500
H	-3.92695200	-2.21548600	-1.90514500
H	-3.86290400	-2.95555200	-0.29082300
C	-5.05123400	-1.17266000	-0.40425500
C	-5.67091500	-0.25331500	-1.28121600
C	-5.58846500	-1.25947500	0.90044800
C	-6.75047100	0.53455200	-0.87915700
H	-5.28686000	-0.15783600	-2.29587900
C	-6.66778500	-0.47293700	1.30599900
H	-5.13933200	-1.95731600	1.60574300
C	-7.26143200	0.43538800	0.42088800
H	-7.19818100	1.23037700	-1.58703300
H	-7.05064800	-0.57191500	2.32058100
H	-8.10243700	1.04890400	0.73557700

Filename: AgCH2PhPPh3SO3_2
Sum of electronic and zero-point Energies = -56525.0995

Figure S46: Cartesian coordinates and energies (eV) for [(R)Ag($PPh_2C_6H_4SO_3$)]$^-$, R = Me, Et, Ph and CH_2Ph.

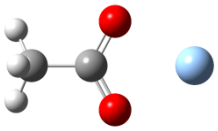


[(Ph)Ag(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

P	0.05629700	0.42839100	-0.06010000
C	-0.29189300	1.53191000	-1.50077600
C	0.68412500	2.48149400	-1.85181500
C	-1.46973800	1.45377600	-2.26005900
C	0.47874300	3.34843400	-2.92644100
H	1.61183000	2.53803300	-1.28632200
C	-1.67038500	2.31976800	-3.34062000
H	-2.23561400	0.72389100	-2.01656200
C	-0.70107300	3.26859400	-3.67458200
H	1.24342000	4.07718200	-3.18463700
H	-2.59021500	2.24725200	-3.91518900
H	-0.86001100	3.93895300	-4.51603600
C	-0.43005600	1.43416200	1.40785100
C	-1.32617600	2.51106600	1.33265700
C	0.11099400	1.08329800	2.65608900
C	-1.68314800	3.21486500	2.48620500
H	-1.75403600	2.79929600	0.37705800
C	-0.24976300	1.78473000	3.80794900
H	0.81495100	0.25714900	2.72722700
C	-1.14832500	2.85288500	3.72501400
H	-2.39069400	4.03696400	2.41489000
H	0.17129800	1.49660800	4.76800700
H	-1.43343900	3.39701500	4.62206800
C	-1.17936500	-0.91957100	-0.15957200
C	-2.53230400	-0.70829800	0.14679100
C	-0.75971100	-2.18341700	-0.61237000
C	-3.46546900	-1.73057800	-0.03805700
H	-2.88302900	0.24570000	0.52923400
C	-1.69361900	-3.21067900	-0.76696900
H	0.28995500	-2.36178300	-0.83491000
C	-3.04592500	-2.98410400	-0.49004500
H	-1.36392100	-4.19051100	-1.10588500
H	-3.78834300	-3.76759800	-0.60962900
S	-5.24170100	-1.36626900	0.21317200
O	-5.59419000	-0.60200200	-1.01984900
O	-5.27219200	-0.55406300	1.46112700
O	-5.88175800	-2.70657800	0.31519800
Ag	2.40015300	-0.27287300	0.01796000
C	4.43614600	-0.82065600	0.07970800
C	4.99598400	-1.73687200	-0.83852700
C	5.32776300	-0.29127400	1.03943400
C	6.34862000	-2.10287800	-0.80630100
H	4.36582200	-2.18432000	-1.60635000
C	6.68283800	-0.64700500	1.08476500
H	4.96362100	0.42114700	1.77900000
C	7.20130100	-1.55771900	0.15881500
H	6.73595600	-2.81438600	-1.53502700
H	7.33312100	-0.21306300	1.84389800
H	8.25264600	-1.83852600	0.18913900

Filename: AgPhPPh3SO3_3
Sum of electronic and zero-point Energies = -55455.8813

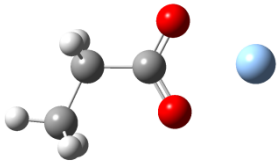
Figure S46 (cont'd): Cartesian coordinates and energies (eV) for [(R)Ag(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$, R = Me, Et, Ph and CH$_2$Ph.



[Ag(O$_2$CMe)]$^-$

O	-0.91416600	1.11737000	-0.01097000
O	-0.91424100	-1.11726200	-0.01097300
C	-1.52216900	0.00008300	-0.01516600
C	-3.04198300	0.00001500	0.00743500
H	-3.43350900	0.90073900	-0.47078800
H	-3.43331200	-0.89694800	-0.47804100
H	-3.37400300	-0.00449600	1.05280000
Ag	1.11176600	-0.00001600	0.00251000

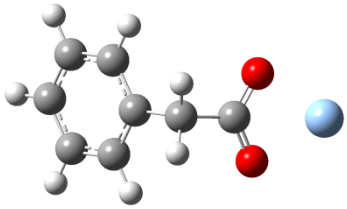
Filename: AgCO2Me_2
Sum of electronic and zero-point Energies = -10216.8276



[Ag(O$_2$CEt)]$^-$

O	-0.34393800	1.31365000	0.00004100
O	-0.71488200	-0.88901800	-0.00013600
C	-1.13049900	0.31051000	-0.00005100
C	-2.63136000	0.59493600	-0.00007800
H	-2.83252100	1.22877100	0.87317600
H	-2.83252600	1.22850400	-0.87352200
Ag	1.47130700	-0.09676300	0.00001400
C	-3.52822300	-0.64369200	0.00011700
H	-4.58407900	-0.34637800	0.00010000
H	-3.34563500	-1.26543300	-0.88222300
H	-3.34559400	-1.26518800	0.88262200

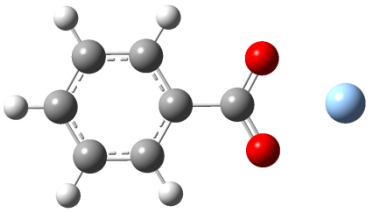
Filename: AgCO2Et
Sum of electronic and zero-point Energies = -11285.8610



[Ag(O$_2$CCH$_2$Ph)]$^-$

O	0.90696400	-0.70609000	1.04349400
O	0.90273600	1.27951300	0.01642700
C	0.38198000	0.42462800	0.79738200
C	-0.95658300	0.76385100	1.46581800
H	-0.98192300	0.26717400	2.44014900
H	-0.99715400	1.84574300	1.61853300
Ag	2.66076400	-0.18319100	-0.37569800
C	-2.13333600	0.31248700	0.61852300
C	-2.77688000	1.20827400	-0.24695700
C	-2.59248800	-1.01176600	0.68168100
C	-3.85843700	0.79311700	-1.02935200
H	-2.42601300	2.23579100	-0.30909800
C	-3.67247800	-1.42976300	-0.10001400
H	-2.09552500	-1.71721200	1.34343900
C	-4.31055200	-0.52773100	-0.95767900
H	-4.34847400	1.50251100	-1.69189300
H	-4.01767200	-2.45894600	-0.03653400
H	-5.15408600	-0.85105400	-1.56256100

Filename: AgCO2CH2Ph
Sum of electronic and zero-point Energies = -16502.0007

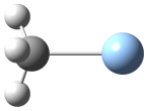


[Ag(O$_2$CPh)]$^-$

O	-0.50312800	-1.11656600	0.00009900
O	-0.50241200	1.11783700	0.00009100
C	0.11023700	0.00051000	0.00006500
Ag	-2.52344500	-0.00014300	-0.00002800
C	1.61088800	0.00014500	0.00001400
C	2.31589700	1.21301700	0.00000000
C	2.31538900	-1.21302300	-0.00000300
C	3.71191800	1.21121500	-0.00002500
H	1.75801000	2.14365500	0.00001600
C	3.71141300	-1.21179700	-0.00002900
H	1.75712100	-2.14343100	0.00001700
C	4.41170300	-0.00043500	-0.00003900
H	4.25412600	2.15350800	-0.00003000
H	4.25323800	-2.15431000	-0.00003600
H	5.49906600	-0.00065900	-0.00005500

Filename: AgCO2Ph
Sum of electronic and zero-point Energies = -15433.0707

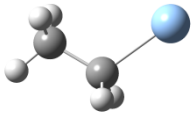
Figure S47: Cartesian coordinates and energies (eV) for [Ag(O$_2$CR)]$^-$, R = Me, Et, Ph and CH$_2$Ph.



[Ag(Me)]⁻

Ag	-0.35745300	0.00000000	0.00000500
C	1.75660300	0.00000500	-0.00001800
H	2.08668600	-0.85912200	-0.58772000
H	2.08679400	0.93854200	-0.45011700
H	2.08720900	-0.07947100	1.03772500

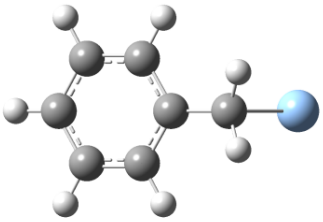
Filename: AgMe
Sum of electronic and zero-point Energies = -5084.9563



[Ag(Et)]⁻

Ag	-0.69859600	-0.04755000	0.00000000
C	1.30914600	0.68320300	0.00000100
H	1.35879300	1.31683200	-0.89054300
H	1.35882600	1.31686000	0.89052200
C	2.37610800	-0.40684400	0.00000000
H	3.38344400	0.04369400	-0.00007900
H	2.31075900	-1.05028600	0.88437800
H	2.31066300	-1.05038400	-0.88429900

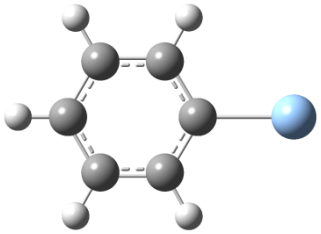
Filename: AgEt
Sum of electronic and zero-point Energies = -6153.8733



[Ag(CH_2Ph)]⁻

Ag	-1.96541500	-0.00001400	-0.23690800
C	-0.36994800	0.00010000	1.21810400
H	-0.58405600	0.89749800	1.80207900
H	-0.58404700	-0.89719500	1.80224400
C	0.97321100	0.00004900	0.59894700
C	1.64432300	1.20643100	0.30800100
C	1.64426400	-1.20638700	0.30809000
C	2.92239000	1.20722200	-0.25042700
H	1.15015000	2.15193700	0.52344600
C	2.92233100	-1.20728100	-0.25033500
H	1.15004800	-2.15185500	0.52360600
C	3.57065500	-0.00005600	-0.53609100
H	3.41640200	2.15292400	-0.46136600
H	3.41629700	-2.15302100	-0.46120900
H	4.56634600	-0.00009600	-0.97183100

Filename: AgCH2Ph
Sum of electronic and zero-point Energies = -11370.2785

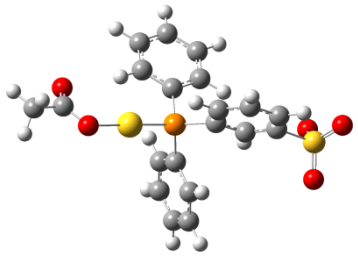


[Ag(Ph)]⁻

Ag	1.66184100	0.00000000	-0.00006200
C	-0.42987300	-0.00000600	0.00039800
C	-1.14420400	1.20821400	0.00022700
C	-1.14420600	-1.20821700	0.00023200
C	-2.54576600	1.20710800	-0.00006300
H	-0.62231100	2.16126000	0.00035300
C	-2.54577000	-1.20710500	-0.00007500
H	-0.62232100	-2.16126500	0.00040700
C	-3.24981900	0.00000200	-0.00023500
H	-3.08340900	2.15319800	-0.00012900
H	-3.08341500	-2.15319200	-0.00016000
H	-4.33723200	0.00000400	-0.00044400

Filename: AgPh
Sum of electronic and zero-point Energies = -10300.9228

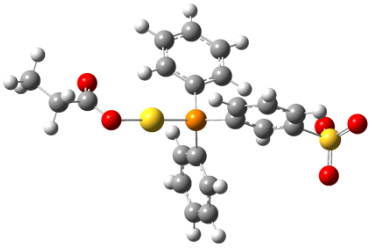
Figure S48: Cartesian coordinates and energies (eV) for $[Ag(R)]^-$, R = Me, Et, Ph and CH_2Ph.



$[(CH_3CO_2)Au(PPh_2C_6H_4SO_3)]^-$

P	0.12073100	0.28996800	0.02288600
C	0.15501100	1.57613200	-1.29668700
C	1.39103600	1.99950600	-1.81249700
C	-1.03174200	2.14529000	-1.79064800
C	1.43820500	2.98787600	-2.80119600
H	2.31569800	1.55267300	-1.45393300
C	-0.97785600	3.12944800	-2.77937700
H	-1.99954400	1.82050600	-1.42064200
C	0.25611500	3.55406500	-3.28456200
H	2.40119100	3.30369000	-3.19446300
H	-1.90319700	3.55720000	-3.15634400
H	0.29334700	4.31821200	-4.05759100
C	-0.36026900	1.18612600	1.55820700
C	-0.05813900	2.54627900	1.72195900
C	-0.95971500	0.48412900	2.61666000
C	-0.35690700	3.19493700	2.92322400
H	0.40382400	3.10388300	0.91250900
C	-1.26272700	1.13721600	3.81239400
H	-1.21277200	-0.56598200	2.50314900
C	-0.96114500	2.49337400	3.96951900
H	-0.12442000	4.25119700	3.03464300
H	-1.74830800	0.58692200	4.61380100
H	-1.20444300	3.00172100	4.89925600
C	-1.26552900	-0.83505700	-0.35995400
C	-2.59554100	-0.45495700	-0.12306100
C	-0.99385700	-2.07738000	-0.96080200
C	-3.64646000	-1.29402100	-0.49726700
H	-2.83939300	0.49134200	0.35022400
C	-2.05035700	-2.91256400	-1.32970100
H	0.03448700	-2.38313800	-1.13584200
C	-3.37487200	-2.52248100	-1.10320500
H	-1.83787200	-3.87213400	-1.79600300
H	-4.20927100	-3.15308300	-1.39553000
S	-5.36425600	-0.76543300	-0.14870600
O	-5.35649700	0.68121000	-0.51088600
O	-5.52023000	-1.02922400	1.30977100
O	-6.19561400	-1.62978200	-1.03061200
O	4.95376700	0.05864200	-0.79254200
O	4.04627900	-1.61394700	0.43095600
C	5.03940900	-0.99257900	-0.14918200
C	6.37870200	-1.70169900	0.03883400
H	7.17714100	-1.14366700	-0.45598500
H	6.60257400	-1.79990700	1.10740600
H	6.32505000	-2.71548500	-0.37481200
Au	2.17140800	-0.70953900	0.22388200

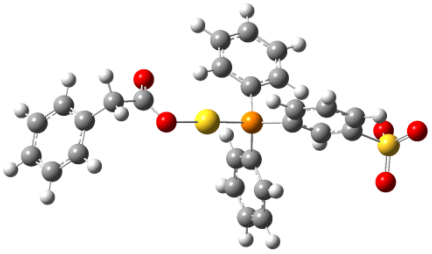
Filename: AuCO2MePPh3SO3_3
Sum of electronic and zero-point Energies = -55066.7188



$[(CH_3CH_2CO_2)Au(PPh_2C_6H_4SO_3)]^-$

P	-0.09639100	0.31538800	0.02918300
C	-0.07341800	1.55584000	-1.33368800
C	1.15983400	1.99654100	-1.84156800
C	-1.26598800	2.07346300	-1.86858900
C	1.19823900	2.95150800	-2.86289000
H	2.08950700	1.58852700	-1.45116200
C	-1.22080000	3.02444400	-2.88973900
H	-2.23121200	1.73390300	-1.50517000
C	0.01016700	3.46682300	-3.38687500
H	2.15930100	3.28113500	-3.24948800
H	-2.15041400	3.41235300	-3.29799300
H	0.04073200	4.20491800	-4.18509500
C	-0.62299700	1.25138100	1.52529300
C	-0.36613700	2.62546200	1.64312900
C	-1.21325200	0.56883000	2.60152000
C	-0.70025300	3.30672300	2.81677500
H	0.08777900	3.16836200	0.81927600
C	-1.55154100	1.25410900	3.76939000
H	-1.43162800	-0.49223100	2.52290900
C	-1.29491900	2.62401800	3.88081200
H	-0.50285700	4.37323100	2.89254300
H	-2.02939800	0.71759600	4.58466600
H	-1.56572800	3.15720000	4.78877200
C	-1.44915400	-0.85588200	-0.33427800
C	-2.79125500	-0.50058100	-0.12941300
C	-1.13879300	-2.11070900	-0.88868400
C	-3.81607100	-1.37690900	-0.49047100
H	-3.06460200	0.45485100	0.30805100
C	-2.16932800	-2.98330200	-1.24410600
H	-0.10090700	-2.39700600	-1.03848600
C	-3.50608600	-2.61805000	-1.05031500
H	-1.92697400	-3.95258700	-1.67435100
H	-4.32076500	-3.27804700	-1.33321600
S	-5.55117500	-0.87779800	-0.18707700
O	-5.57236500	0.55365000	-0.60489700
O	-5.72313000	-1.08912800	1.27809900
O	-6.34797700	-1.79540500	-1.04680700
O	4.75875900	0.17166800	-0.70177100
O	3.86516400	-1.47971800	0.55907700
C	4.85545100	-0.85662900	-0.02428700
C	6.20675000	-1.54105200	0.21401700
H	6.35061500	-1.61600600	1.30029200
H	6.11767000	-2.57662400	-0.14107200
Au	1.97421200	-0.62663800	0.29425500
C	7.39216100	-0.83693700	-0.44735000
H	8.32652300	-1.37541100	-0.24032700
H	7.25946900	-0.77847900	-1.53297600
H	7.49552900	0.18959400	-0.07955500

Filename: AuCO2EtPPh3SO3_2
Sum of electronic and zero-point Energies = -56135.7566

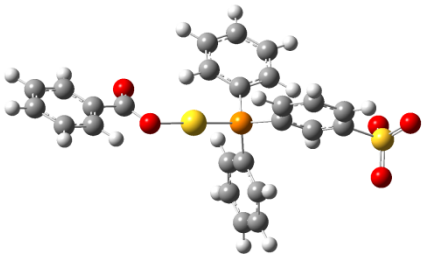


$[(PhCH_2CO_2)Au(PPh_2C_6H_4SO_3)]^-$

P	-0.89370800	0.33504500	0.04297700
C	-1.06247400	2.06477600	-0.56892500
C	0.08207800	2.76240000	-0.98806000
C	-2.31583900	2.69963000	-0.61716100
C	-0.02517500	4.08281400	-1.43712000
H	1.05413000	2.27454800	-0.97699500
C	-2.41646000	4.01681300	-1.06863700
H	-3.21713500	2.17316400	-0.31756000
C	-1.27213900	4.71132100	-1.47650900
H	0.86788100	4.61041400	-1.76240000
H	-3.39218600	4.49416300	-1.10583500
H	-1.35557900	5.73608000	-1.83108800
C	-1.17691700	0.43274300	1.85982900
C	-0.87923300	1.60402600	2.57233100
C	-1.61393600	-0.70398000	2.55946500
C	-1.02267000	1.63908900	3.96197100
H	-0.54171900	2.49228300	2.04644400
C	-1.76262300	-0.66257100	3.94661500
H	-1.86201300	-1.61530600	2.02319800
C	-1.46613300	0.50782000	4.65155600
H	-0.79522400	2.55509400	4.50167900
H	-2.12460900	-1.54233100	4.47176600
H	-1.58865600	0.53954000	5.73134500
C	-2.29724800	-0.61196700	-0.63941800
C	-3.58705600	-0.48263800	-0.10262300
C	-2.09059900	-1.43134000	-1.76411300
C	-4.66565300	-1.14637800	-0.69013500
H	-3.77734600	0.13086900	0.77275000
C	-3.17362300	-2.09481400	-2.34370100
H	-1.09190400	-1.54542800	-2.17794800
C	-4.46033400	-1.95122300	-1.81222000
H	-3.01199800	-2.72690800	-3.21414400
H	-5.31679000	-2.44946100	-2.25672500
S	-6.32720900	-0.95401400	0.05404200
O	-6.41789000	0.51302700	0.30642000
O	-6.25255000	-1.78262300	1.29048700
O	-7.25459900	-1.47098700	-0.98925500
O	3.76288900	0.75606200	-1.54150600
O	3.08031400	-1.28903800	-0.85007200
C	3.95453300	-0.44246000	-1.31579600
C	5.34109100	-1.06774500	-1.57242200
H	5.23062500	-2.14801800	-1.70152200
H	5.72180400	-0.63895400	-2.50594800
Au	1.18102700	-0.50218000	-0.44643500
C	6.30822500	-0.77534000	-0.44167000
C	6.93140500	0.47861400	-0.33756500
C	6.58710900	-1.74261400	0.53488800
C	7.81065500	0.75568500	0.71206900
H	6.70770300	1.24253200	-1.07782200
C	7.46685700	-1.46899400	1.58695100
H	6.10312500	-2.71479600	0.47286800
C	8.08395000	-0.21808700	1.67891400
H	8.28137200	1.73435100	0.77644800
H	7.66757300	-2.23310900	2.33476200
H	8.76871800	-0.00295900	2.49609100

Filename: AuCO2CH2PhPPh3SO3_3
Sum of electronic and zero-point Energies = -61351.9161

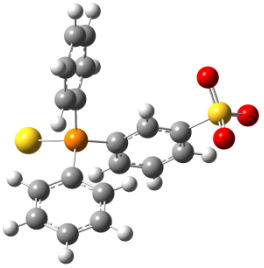
Figure S49: Cartesian coordinates and energies (eV) for $[(RCO_2)Au(PPh_2C_6H_4SO_3)]^-$, R = Me, Et, Ph and CH_2Ph.



[(PhCO$_2$)Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

P	-0.75869000	0.42235400	0.05693200
C	-0.94139000	1.86616200	-1.07322000
C	0.20575400	2.55732100	-1.49679700
C	-2.20710400	2.29330100	-1.51078300
C	0.08604200	3.66832300	-2.33793500
H	1.19221700	2.22441100	-1.18183900
C	-2.31947700	3.40139500	-2.35264500
H	-3.10656300	1.76338700	-1.21203200
C	-1.17472200	4.09199500	-2.76551200
H	0.98193000	4.19211100	-2.66163300
H	-3.30367300	3.71764900	-2.68821900
H	-1.26662900	4.95237500	-3.42437900
C	-1.32735100	1.02213700	1.70295200
C	-1.19968800	2.37386900	2.05634600
C	-1.81288500	0.10740300	2.65143500
C	-1.55717500	2.80400900	3.33693700
H	-0.82721600	3.09423700	1.33389000
C	-2.17551700	0.54241900	3.92724200
H	-1.93155500	-0.94032300	2.39141000
C	-2.04706600	1.89066500	4.27398600
H	-1.45992400	3.85539500	3.59619200
H	-2.57228600	-0.17264700	4.64283100
H	-2.33612400	2.22818900	5.26620600
C	-1.97127000	-0.83336300	-0.47516900
C	-3.33682600	-0.69063100	-0.18607600
C	-1.53383400	-1.92624600	-1.24550500
C	-4.26184100	-1.61518300	-0.67459900
H	-3.70521700	0.13399100	0.41671500
C	-2.46451000	-2.84858000	-1.72735700
H	-0.47591700	-2.04946500	-1.46298800
C	-3.82699900	-2.69348800	-1.44752100
H	-2.12415900	-3.69210700	-2.32396200
H	-4.56687000	-3.39372300	-1.82381600
S	-6.03090700	-1.39066000	-0.26020400
O	-6.25319900	0.06459300	-0.49887100
O	-6.10600000	-1.79261500	1.17285000
O	-6.74252300	-2.29789800	-1.20148900
O	4.05917100	1.05795200	-0.64459300
O	3.41015700	-0.92843700	0.21914800
C	4.29960600	-0.07327200	-0.20454600
Au	1.41810400	-0.28102700	0.12238400
C	5.72596000	-0.57280000	-0.12253000
C	6.76904200	0.26543100	-0.54120300
C	6.02780100	-1.85431000	0.36070600
C	8.09465300	-0.16943000	-0.47841300
H	6.51730500	1.25407700	-0.91256400
C	7.35402100	-2.29044000	0.42301600
H	5.21406300	-2.49576400	0.68241100
C	8.39068700	-1.44947700	0.00397300
H	8.89702900	0.48843000	-0.80540700
H	7.57892500	-3.28643000	0.79828500
H	9.42302200	-1.78945200	0.05282900

Filename: AuCO2PhPPh3SO3_3
Sum of electronic and zero-point Energies = -60282.9972

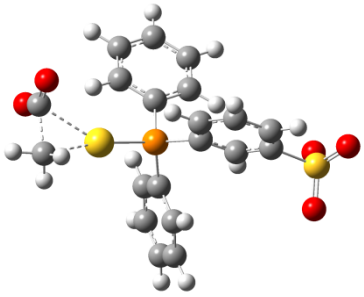


[Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

P	-0.72440600	-0.00714900	0.08841900
C	-1.13946200	-1.19271300	1.41085700
C	-2.46571500	-1.37235800	1.83697000
C	-0.09780400	-1.90307300	2.03368600
C	-2.74781200	-2.24739400	2.88670900
H	-3.27625200	-0.83878400	1.34629000
C	-0.39060100	-2.77501900	3.08503700
H	0.93157100	-1.78026000	1.71009600
C	-1.71032400	-2.94836500	3.51109900
H	-3.77540400	-2.38615700	3.21104100
H	0.41811300	-3.31900700	3.56439500
H	-1.93208200	-3.63326800	4.32497300
C	-0.47647500	1.63553300	0.82122900
C	-0.85157600	1.90037500	2.14899000
C	0.09845800	2.65246700	0.03596000
C	-0.63964400	3.17094300	2.68764800
H	-1.28674200	1.12032800	2.76557400
C	0.31136100	3.91482000	0.58529100
H	0.40542100	2.45401400	-0.98698800
C	-0.05803900	4.17560700	1.90978200
H	-0.91603100	3.36872400	3.71937700
H	0.78128700	4.68816200	-0.01485700
H	0.11811800	5.15889600	2.33678300
C	0.78257300	-0.52511600	-0.74665700
C	2.01342500	-0.07568300	-0.24137000
C	0.73992400	-1.45831000	-1.80233100
C	3.20195600	-0.57695200	-0.77352400
H	2.07675100	0.65114200	0.56231000
C	1.93598100	-1.93190800	-2.33723500
H	-0.21232400	-1.79938900	-2.20130300
C	3.16561900	-1.49695800	-1.82173200
H	1.91201300	-2.63925300	-3.16223500
H	4.10696500	-1.85314800	-2.23019000
S	4.77392200	-0.03801200	0.00442100
O	4.75224300	-0.80229900	1.28215700
O	4.57811800	1.42797900	0.16141600
O	5.81145500	-0.45085100	-0.97112900
Au	-2.48143900	0.08163800	-1.41144700

Filename: AuPPh3SO3
Sum of electronic and zero-point Energies = -48845.2930

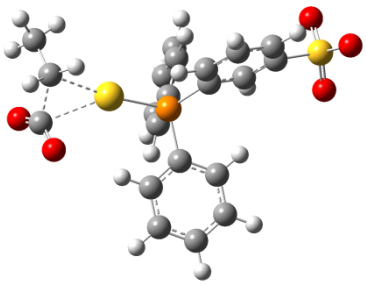
Figure S49 (cont'd): Cartesian coordinates and energies (eV) for [(RCO$_2$)Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$, R = Me, Et, Ph and CH$_2$Ph, and for [Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$.



TS $[(CH_3CO_2)Au(PPh_2C_6H_4SO_3)]^- \rightarrow [(CH_3)Au(PPh_2C_6H_4SO_3)]^-$
(-351 cm^{-1})

O	-4.85596700	-0.00972900	0.42291000
C	-4.54050500	-1.20533700	0.36853100
O	-4.54046000	-2.17248100	1.12203400
C	-4.15371900	-1.73027600	-1.30976600
H	-3.66261100	-2.70373300	-1.40513000
H	-5.22437000	-1.90678700	-1.46208400
H	-3.90082500	-1.04387900	-2.13786300
P	-0.19152800	0.32448900	0.00696900
Au	-2.21195400	-0.66179000	-0.47534700
C	0.32430100	1.46897800	-1.33662300
C	0.96514300	0.96022000	-2.47840100
C	0.01599300	2.83611700	-1.27232100
C	1.30361300	1.81097900	-3.53154300
H	1.22466400	-0.09275100	-2.53813600
C	0.35051700	3.68265800	-2.33267300
H	-0.47745000	3.24416400	-0.39520100
C	0.99598800	3.17325700	-3.46216500
H	1.82229100	1.40907700	-4.39761800
H	0.11358800	4.74169600	-2.26838000
H	1.26722200	3.83514500	-4.28078200
C	-0.32368900	1.35843900	1.52207800
C	0.83223400	1.83844600	2.16273500
C	-1.58873000	1.67557600	2.04236500
C	0.71804100	2.63498600	3.30319500
H	1.82008000	1.58781500	1.78738300
C	-1.69495500	2.47512300	3.18495000
H	-2.49097200	1.29352700	1.57038100
C	-0.54448700	2.95582700	3.81465800
H	1.61822200	2.99636700	3.79334800
H	-2.67936200	2.70830000	3.58209700
H	-0.62859900	3.57170400	4.70696400
C	1.18358800	-0.84527800	0.25357200
C	0.90485400	-2.16003900	0.66923200
C	2.51484500	-0.43002500	0.09819600
C	1.95903500	-3.03589300	0.93433400
H	-0.12434600	-2.48993500	0.78656500
C	3.56252100	-1.31369200	0.36274700
H	2.76265000	0.57600700	-0.22635600
C	3.28562100	-2.61597300	0.78326400
H	1.74291500	-4.05108300	1.25924700
H	4.11770400	-3.28136900	0.99360000
S	5.28182000	-0.73765600	0.10864900
O	5.26914000	0.63675900	0.68646400
O	5.44125400	-0.77602600	-1.37262800
O	6.10929200	-1.72630200	0.85162700

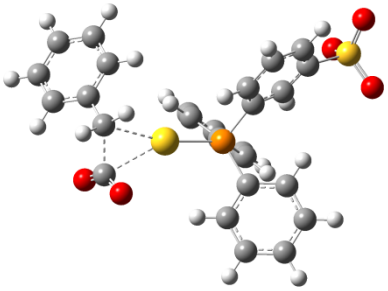
Filename: TS_AuCO2MePPh3SO3_3
Sum of electronic and zero-point Energies = -55064.8026



TS $[(CH_3CH_2CO_2)Au(PPh_2C_6H_4SO_3)]^- \rightarrow [(CH_3CH_2)Au(PPh_2C_6H_4SO_3)]^-$
(-372 cm^{-1})

O	-4.43795500	0.46775400	-1.31366700
C	-4.60174200	-0.21161100	-0.29261600
O	-5.15017400	-0.09258100	0.79215300
C	-4.08008900	-1.97932000	-0.55118700
H	-4.92726900	-2.05343500	-1.24233600
H	-3.26039200	-2.33477600	-1.21850600
P	-0.05067100	0.32613700	0.03834800
C	0.30086300	0.56657500	1.82629800
C	-0.08886800	1.74894300	2.47363600
C	0.88446000	-0.46863100	2.57459500
C	0.11018900	1.89559800	3.84852300
H	-0.54349700	2.55726700	1.90843400
C	1.08737100	-0.31441600	3.94693300
H	1.20315800	-1.38558900	2.08787200
C	0.70013600	0.86651000	4.58702900
H	-0.19164800	2.81784800	4.33844900
H	1.56166100	-1.11371700	4.50979500
H	0.86405600	0.98611900	5.65503200
C	-0.03218200	2.00964500	-0.70536200
C	1.17222100	2.72453200	-0.83125200
C	-1.23243300	2.58907400	-1.14760000
C	1.16935900	4.00625000	-1.38341300
H	2.11414900	2.28768700	-0.51328900
C	-1.22729600	3.87506400	-1.69823300
H	-2.16960000	2.04188600	-1.07668300
C	-0.02979200	4.58419700	-1.81566000
H	2.10714300	4.54696900	-1.48020200
H	-2.16245500	4.31146700	-2.03928500
H	-0.02700200	5.58180700	-2.24861400
C	1.36376400	-0.59345800	-0.65583700
C	1.14644900	-1.50223500	-1.70691700
C	2.67036600	-0.35556200	-0.20246600
C	2.23359800	-2.14896500	-2.29765100
H	0.13627500	-1.69675400	-2.05819800
C	3.75211600	-1.00659300	-0.79780100
H	2.87323100	0.33298800	0.61207100
C	3.53510600	-1.90164200	-1.84735100
H	2.06334600	-2.84906700	-3.11256500
H	4.39368300	-2.38697900	-2.30190600
S	5.43502700	-0.69133800	-0.14874700
O	5.48416600	-1.51460700	1.09236400
O	6.33563800	-1.15283200	-1.23984400
O	5.43717300	0.77992000	0.09210800
C	-4.26736500	-2.88587900	0.66383800
H	-4.68827900	-3.86125600	0.37901400
H	-3.32419200	-3.07334600	1.18991100
H	-4.95198800	-2.40649800	1.37102300
Au	-2.10150500	-0.67117600	-0.28183800

Filename: TS_AuCO2EtPPh3SO3_2
Sum of electronic and zero-point Energies = -56133.7615

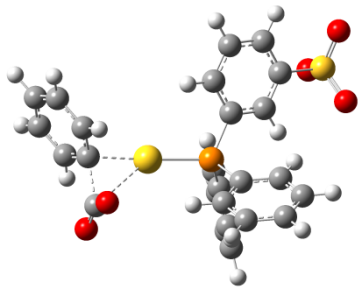


TS $[(PhCH_2CO_2)Au(PPh_2C_6H_4SO_3)]^- \rightarrow [(PhCH_2)Au(PPh_2C_6H_4SO_3)]^-$
(-337 cm^{-1})

O	-3.64721200	2.36200100	-1.14907000
C	-4.03384900	1.42309900	-0.44174800
O	-4.61251700	1.26579800	0.62100700
C	-3.88577400	-0.18142400	-1.37782000
H	-4.75691800	0.15806800	-1.94883600
H	-3.12636400	-0.30381500	-2.17451200
P	0.50792100	0.66057200	0.14832800
C	0.65797100	0.13644600	1.90127000
C	1.59853800	0.71689600	2.76570100
C	-0.16559700	-0.89930200	2.37206400
C	1.72178600	0.25657200	4.07896300
H	2.23845700	1.52303300	2.42005800
C	-0.03843500	-1.35566400	3.68467000
H	-0.91066700	-1.34400300	1.71746100
C	0.90659300	-0.78017600	4.53928800
H	2.46289700	0.70415400	4.73573000
H	-0.68099600	-2.15783900	4.03762300
H	1.00745100	-1.13911900	5.56040200
C	1.12822100	2.39020800	0.07373000
C	2.48117900	2.67538400	-0.17316700
C	0.22381400	3.44566500	0.28091200
C	2.92280700	4.00159700	-0.19509400
H	3.19254200	1.87510100	-0.35507500
C	0.67210600	4.76779500	0.25954900
H	-0.83167000	3.23896500	0.43955600
C	2.02205000	5.04754700	0.02370300
H	3.97214900	4.20926200	-0.38719700
H	-0.03786600	5.57602200	0.41445900
H	2.36860800	6.07800000	0.00080900
C	1.67697900	-0.35292500	-0.81816600
C	1.39357600	-0.63704600	-2.16651800
C	2.89244000	-0.77098100	-0.25768400
C	2.33167500	-1.32389200	-2.93838900
H	0.44801800	-0.32498200	-2.60328300
C	3.83829100	-1.43139000	-1.04584700
H	3.12679200	-0.59380500	0.78763800
C	3.55664300	-1.71302500	-2.38371000
H	2.10719600	-1.55350400	-3.97768200
H	4.30258100	-2.24117100	-2.97018800
S	5.47525900	-1.81468600	-0.32060300
O	5.15109000	-2.37707100	1.01901700
O	6.08580800	-2.77332200	-1.28085500
O	6.12757000	-0.47314300	-0.27756800
C	-4.16285800	-1.46971200	-0.66510800
C	-5.33529900	-1.64074900	0.09310400
C	-3.26823900	-2.55401700	-0.74349000
C	-5.59797900	-2.84699400	0.74725400
H	-6.02828000	-0.81091600	0.18655400
C	-3.52889500	-3.76116000	-0.09061400
H	-2.35489000	-2.45192300	-1.32720500
C	-4.69815300	-3.91444500	0.66143200
H	-6.51016400	-2.95069500	1.33121500
H	-2.81838200	-4.58081000	-0.17229100
H	-4.90410400	-4.85188400	1.17289400
Au	-1.67322500	0.52739600	-0.56391600

Filename: TS_AuCO2CH2PhPPh3SO3_2
Sum of electronic and zero-point Energies = -61350.0157

Figure S50: Cartesian coordinates and transition state energies (eV) for decarboxylation from $[(RCO_2)Au(P^*)]^-$ (R = Me, Et, Ph, CH_2Ph).

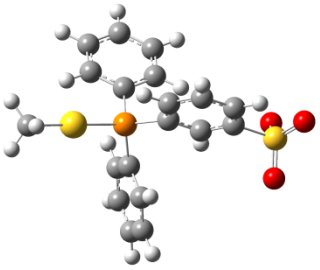


TS $[(PhCO_2)Au(PPh_2C_6H_4SO_3)]^- \rightarrow [(Ph)Au(PPh_2C_6H_4SO_3)]^-$
(-267 cm^{-1})

O	-4.41587800	1.29716500	-1.30378300
C	-4.38802500	0.96555600	-0.13101600
O	-4.62800300	1.38308000	0.98592800
P	0.39641100	0.55672200	0.00410700
C	0.91703800	1.17604200	1.65642200
C	0.78459000	2.53423400	1.98317400
C	1.36588100	0.27411700	2.63496500
C	1.10428700	2.98372600	3.26672400
H	0.43723100	3.24400900	1.23807900
C	1.69042700	0.72894900	3.91420900
H	1.48656800	-0.77851800	2.39653200
C	1.55949200	2.08358100	4.23370100
H	1.00258000	4.03932800	3.50589000
H	2.05945000	0.02383500	4.65409900
H	1.81834800	2.43627700	5.22893500
C	0.65286800	1.96882900	-1.15104200
C	1.94612700	2.37799000	-1.52113300
C	-0.46063400	2.65274100	-1.66456400
C	2.11694800	3.46140300	-2.38465000
H	2.82200700	1.85331400	-1.15173100
C	-0.28320700	3.73899500	-2.52756400
H	-1.46705400	2.33581300	-1.40247600
C	1.00402100	4.14478400	-2.88739600
H	3.12190900	3.76432800	-2.66669300
H	-1.15468900	4.25711600	-2.91933800
H	1.14187600	4.98608500	-3.56257900
C	1.59094000	-0.74298900	-0.46023800
C	1.14646500	-1.84228500	-1.21683800
C	2.95053700	-0.63204200	-0.13025800
C	2.06434900	-2.80319800	-1.64568700
H	0.09293100	-1.94159900	-1.46579800
C	3.86223800	-1.59592800	-0.56375300
H	3.32524400	0.19709300	0.46217700
C	3.42049600	-2.68071400	-1.32428700
H	1.71849100	-3.65114400	-2.23276700
H	4.15050100	-3.41126100	-1.66006400
S	5.62133900	-1.42405200	-0.08585400
O	5.64352400	-1.89769200	1.32690600
O	6.34476400	-2.29911300	-1.04825600
O	5.87704700	0.03614300	-0.24603100
C	-3.89667600	-0.87333300	-0.00930300
C	-4.11674700	-1.62159600	-1.19181500
C	-4.19679300	-1.50064600	1.22521800
C	-4.57271000	-2.94040300	-1.14447200
H	-3.95695300	-1.13174300	-2.14910500
C	-4.64869900	-2.81979800	1.27942700
H	-4.10139300	-0.91747700	2.13756900
C	-4.83425100	-3.54107400	0.09298300
H	-4.73683800	-3.49689100	-2.06487900
H	-4.86964800	-3.28426400	2.23813300
H	-5.19851200	-4.56555700	0.13255300
Au	-1.83322800	-0.13497500	0.01112100

Filename: TS_AuCO2PhPPh3SO3_2
Sum of electronic and zero-point Energies = -60281.5175

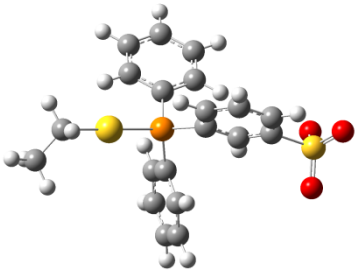
Figure S50 (cont'd): Cartesian coordinates and transition state energies (eV) for decarboxylation from $[(RCO_2)Au(P^*)]^-$ (R = Me, Et, Ph, CH_2Ph).



[(Me)Au($PPh_2C_6H_4SO_3$)]$^-$

P	0.59670300	0.20082700	-0.01317200
C	0.61351500	1.66782800	-1.13775100
C	1.85308800	2.17658900	-1.55834800
C	-0.56601100	2.29142500	-1.57899200
C	1.91530800	3.29714900	-2.39264900
H	2.76907700	1.68537600	-1.23876800
C	-0.50113000	3.40812900	-2.41596100
H	-1.53796200	1.90838200	-1.28309500
C	0.73773100	3.91499700	-2.82243300
H	2.88271000	3.67841600	-2.71139100
H	-1.42303300	3.87662000	-2.75093000
H	0.78353100	4.78284800	-3.47649100
C	0.22369600	0.90752600	1.65021300
C	0.49258700	2.24819900	1.96283900
C	-0.25616200	0.05635600	2.66021200
C	0.28018400	2.72985600	3.25833500
H	0.85895300	2.92382500	1.19557300
C	-0.47461600	0.54130100	3.95017900
H	-0.48165100	-0.98241200	2.43525600
C	-0.20547100	1.87961700	4.25425700
H	0.48419400	3.77434000	3.48228600
H	-0.86878900	-0.12505200	4.71301700
H	-0.38319900	2.25781800	5.25805400
C	-0.89668300	-0.75656400	-0.46881200
C	-2.18585000	-0.34611700	-0.09707800
C	-0.73826600	-1.90540300	-1.26580600
C	-3.30748400	-1.05270400	-0.53734500
H	-2.33898500	0.52626300	0.53138700
C	-1.86326700	-2.61330300	-1.69358800
H	0.25889800	-2.23805400	-1.54337500
C	-3.14733100	-2.18621300	-1.33652500
H	-1.73731600	-3.50150400	-2.30933300
H	-4.03570400	-2.71345800	-1.67131200
S	-4.97070800	-0.46191400	-0.05217400
O	-4.92162200	0.99365400	-0.37638200
O	-5.04292100	-0.75905400	1.40640300
O	-5.90209800	-1.25955500	-0.89771100
Au	2.65151500	-1.02957600	-0.03678400
C	4.44104500	-2.09873200	-0.03741400
H	4.96078800	-1.98724200	0.92380200
H	4.25283800	-3.16819200	-0.20243200
H	5.11054100	-1.74324400	-0.83243300

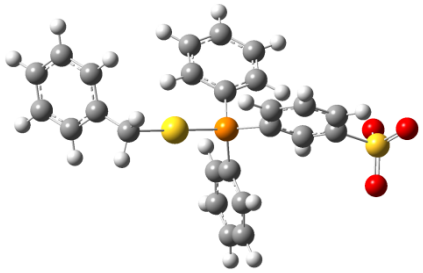
Filename: AuMePPh3SO3_3
Sum of electronic and zero-point Energies = -49934.7915



[(Et)Au($PPh_2C_6H_4SO_3$)]$^-$

P	0.41684800	0.29217100	-0.02538900
C	0.31467300	1.90406500	-0.92479100
C	1.50905600	2.53084200	-1.31556000
C	-0.91107700	2.52277800	-1.22438100
C	1.48183600	3.76100000	-1.98025100
H	2.46001300	2.04654000	-1.10669200
C	-0.93565500	3.74943300	-1.89239100
H	-1.84993400	2.05178200	-0.94932400
C	0.25890900	4.37241200	-2.26929200
H	2.41517800	4.23331100	-2.27796100
H	-1.89230700	4.21290800	-2.11958600
H	0.23497300	5.32612000	-2.79170900
C	0.06580500	0.73081400	1.73207800
C	0.30295500	2.01994600	2.23203700
C	-0.35705600	-0.27512100	2.61755200
C	0.11510700	2.29918600	3.58913700
H	0.62518000	2.81282400	1.56339000
C	-0.55090700	0.00803100	3.97017500
H	-0.55814800	-1.27681300	2.24802300
C	-0.31380800	1.29585300	4.46113300
H	0.29377500	3.30607500	3.95926000
H	-0.90143900	-0.77611500	4.63617900
H	-0.47246500	1.51664900	5.51389600
C	-1.03696000	-0.67623100	-0.57609800
C	-2.33401700	-0.40009300	-0.11753800
C	-0.84189100	-1.68901200	-1.53334300
C	-3.42859600	-1.10340200	-0.62560800
H	-2.51501900	0.36441600	0.63225100
C	-1.93962000	-2.39458500	-2.03047700
H	0.16232100	-1.91910000	-1.88071300
C	-3.23263900	-2.10029100	-1.58335000
H	-1.78518100	-3.17682900	-2.77085400
H	-4.10090900	-2.62660100	-1.96856800
S	-5.10422600	-0.69342900	-0.01331100
O	-5.13895500	0.79623000	-0.08878000
O	-5.11722700	-1.23378200	1.37558300
O	-6.01899100	-1.38903700	-0.96090200
Au	2.54061300	-0.80264400	-0.28338700
C	4.39213500	-1.76294700	-0.50484900
H	4.19499400	-2.79508600	-0.83094200
H	4.92741200	-1.27894200	-1.33553900
C	5.28950100	-1.78089200	0.74605000
H	5.53733500	-0.76634100	1.08395000
H	4.80216200	-2.28785700	1.58856600
H	6.24340600	-2.30379000	0.55918500

Filename: AuEtPPh3SO3_3
Sum of electronic and zero-point Energies = -51003.6629

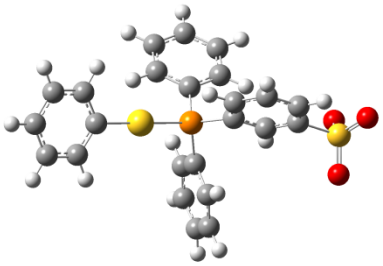


[($PhCH_2$)Au($PPh_2C_6H_4SO_3$)]$^-$

P	0.31998200	0.26799700	-0.01517800
C	0.22931500	1.33239700	1.49146700
C	-1.03362100	1.70759200	1.97753200
C	1.38156800	1.78115000	2.15961500
C	-1.14491400	2.52854400	3.10414600
H	-1.93066200	1.34771700	1.47940300
C	1.26682300	2.59784700	3.28689500
H	2.36964500	1.49129200	1.81488700
C	0.00532300	2.97531900	3.75980000
H	-2.12990700	2.80848000	3.46986900
H	2.16710600	2.93347900	3.79521200
H	-0.07921800	3.60889900	4.63978400
C	0.83424000	1.41568100	-1.36366000
C	0.56528300	2.79101000	-1.29855500
C	1.42002000	0.88959700	-2.52747800
C	0.88261800	3.62541600	-2.37447700
H	0.11618500	3.21711900	-0.40614500
C	1.74177500	1.72613100	-3.59717300
H	1.64811000	-0.17066000	-2.59179800
C	1.47265400	3.09649400	-3.52488200
H	0.67680200	4.69099000	-2.30562300
H	2.21672500	1.30680800	-4.48023100
H	1.73087700	3.74801300	-4.35614600
C	1.74284100	-0.85357600	0.23863700
C	3.06809800	-0.41310400	0.10394000
C	1.49019800	-2.17940100	0.63672400
C	4.13115700	-1.27352400	0.38703100
H	3.29601200	0.59897600	-0.21705900
C	2.55779300	-3.03667700	0.91040400
H	0.46559700	-2.53137200	0.72849100
C	3.87718800	-2.58542300	0.79159300
H	2.35905200	-4.06110500	1.21836800
H	4.72115600	-3.23199300	1.01288700
S	5.84288900	-0.64930900	0.20992000
O	5.80089100	0.66247200	0.91891900
O	6.02787200	-0.53955700	-1.26480800
O	6.68010100	-1.69055300	0.86768800
Au	-1.75320900	-0.81029400	-0.50245100
C	-3.59930700	-1.74163100	-0.94527000
H	-3.69052700	-1.76446900	-2.03834000
H	-3.52834000	-2.77856300	-0.59413500
C	-4.77330800	-1.05001300	-0.32777700
C	-5.24236200	-1.39702900	0.95612800
C	-5.46128900	-0.02018800	-1.00247600
C	-6.33299800	-0.74750000	1.53808000
H	-4.73282200	-2.18730500	1.50495900
C	-6.55239800	0.63230500	-0.42485400
H	-5.12444600	0.27288100	-1.99547000
C	-6.99878900	0.27542000	0.85287200
H	-6.66580800	-1.04274600	2.53164700
H	-7.05813600	1.42306300	-0.97629800
H	-7.84827600	0.78279100	1.30431700

Filename: AuCH2PhPPh3SO3_2
Sum of electronic and zero-point Energies = -56220.11917

Figure S51: Cartesian coordinates and energies (eV) for [(R)Au($PPh_2C_6H_4SO_3$)]$^-$, R = Me, Et, Ph and CH_2Ph.

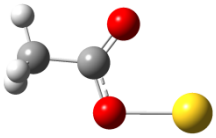


[(Ph)Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

P	-0.17852300	0.48914100	-0.01559200
C	-0.48581600	1.89187200	-1.17755000
C	0.60796900	2.65978300	-1.60943000
C	-1.77414400	2.21926600	-1.63349000
C	0.41780700	3.74502200	-2.47045300
H	1.61027800	2.39992700	-1.27725700
C	-1.96023200	3.30125900	-2.49734600
H	-2.63526500	1.63232500	-1.32894600
C	-0.86709400	4.06737700	-2.91553600
H	1.27469100	4.32925200	-2.79756000
H	-2.96266200	3.53914000	-2.84375900
H	-1.01649700	4.90710300	-3.59038400
C	-0.69621700	1.13255400	1.63360300
C	-0.70956100	2.50619300	1.91708200
C	-0.99809200	0.22115900	2.65950200
C	-1.02416000	2.96023300	3.20149700
H	-0.48448400	3.22642400	1.13600300
C	-1.31839000	0.67763800	3.93871700
H	-1.00638500	-0.84601500	2.45586400
C	-1.33079600	2.04860200	4.21434700
H	-1.03988300	4.02857500	3.40376800
H	-1.57234700	-0.03951000	4.71484700
H	-1.58798700	2.40280500	5.20958600
C	-1.40644100	-0.79900100	-0.43857400
C	-2.75902400	-0.67227000	-0.08774500
C	-0.98537300	-1.91299700	-1.18798100
C	-3.68940000	-1.62705300	-0.50352100
H	-3.11109300	0.16718200	0.50453300
C	-1.91923100	-2.86994900	-1.59048600
H	0.06398900	-2.02622500	-1.44869400
C	-3.27049900	-2.72625200	-1.25573700
H	-1.59077700	-3.73080000	-2.16900800
H	-4.01466500	-3.45059400	-1.57331000
S	-5.44743200	-1.40270200	-0.04538800
O	-5.70715900	0.02473300	-0.39315400
O	-5.47233900	-1.68814100	1.41692300
O	-6.17253200	-2.39409700	-0.88731200
Au	2.09861600	-0.22839300	-0.01955400
C	4.07465800	-0.83071700	-0.01032400
C	4.78140200	-1.08037500	-1.20662900
C	4.79149800	-1.01149200	1.19243700
C	6.12204200	-1.48598300	-1.20638200
H	4.27808300	-0.95829500	-2.16390000
C	6.13208700	-1.41677200	1.20368100
H	4.29631700	-0.83428400	2.14515200
C	6.80559400	-1.65632600	0.00164900
H	6.63211200	-1.66993800	-2.15106500
H	6.65022000	-1.54627900	2.15297400
H	7.84714900	-1.97224600	0.00638500

Filename: AuPhPPh3SO3_2
Sum of electronic and zero-point Energies = -55150.9758

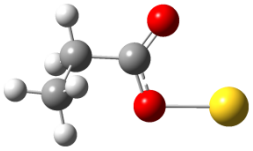
Figure S51 (cont'd): Cartesian coordinates and energies (eV) for [(R)Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$, R = Me, Et, Ph and CH$_2$Ph.



[Au(O$_2$CMe)]$^-$

O	-1.66565100	1.32476800	-0.00455500
O	-1.08329400	-0.85448000	-0.01375600
C	-1.95646300	0.13074600	-0.00905900
C	-3.39744400	-0.36588400	0.00752600
H	-4.07311100	0.47720400	-0.14568200
H	-3.55130500	-1.12343700	-0.76620600
H	-3.60692300	-0.83185700	0.97659900
Au	0.82716900	-0.01105600	0.00115200

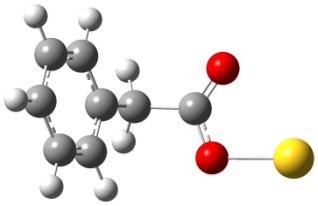
Filename: AuCO2Me
Sum of electronic and zero-point Energies = -9910.3440



[Au(O$_2$CEt)]$^-$

O	1.23253600	1.62497500	-0.28039800
O	0.89785100	-0.51445900	0.35765700
C	1.64864400	0.54058700	0.11574200
C	3.13169200	0.27261300	0.39827500
H	3.67039200	1.19530100	0.16618900
H	3.23068500	0.08432100	1.47482900
C	3.69994600	-0.91652400	-0.39004000
H	4.76291300	-1.04810300	-0.15671300
H	3.17350800	-1.84224500	-0.13968200
H	3.61135600	-0.75382000	-1.47047600
Au	-1.09333700	-0.07467900	-0.01564700

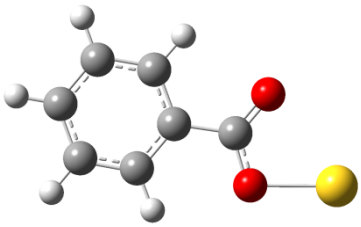
Filename: AuCO2Et
Sum of electronic and zero-point Energies = -10979.3524



[Au(O$_2$CCH$_2$Ph)]$^-$

O	-0.07962400	1.77658000	-0.54202700
O	-0.34896600	0.03281100	0.87129100
C	0.30101400	1.06424900	0.37902400
C	1.64612900	1.29307900	1.09952500
H	1.87043900	2.35922800	1.01128700
H	1.52166200	1.04445600	2.15748600
C	2.76256400	0.46551100	0.49148600
C	2.92095800	-0.88612400	0.83411300
C	3.65665200	1.03949100	-0.42323100
C	3.95289900	-1.64484800	0.27785000
H	2.22763500	-1.34381900	1.53575100
C	4.69202500	0.28246600	-0.97959300
H	3.54092100	2.08467400	-0.70059200
C	4.84359100	-1.06211800	-0.63034300
H	4.06376500	-2.69020700	0.55548400
H	5.37946500	0.74472700	-1.68364100
H	5.64936800	-1.65155000	-1.06046100
Au	-2.14531000	-0.23206200	-0.13598000

Filename: AuCO2CH2Ph
Sum of electronic and zero-point Energies = -16195.5138

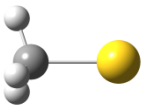


[Au(O$_2$CPh)]$^-$

O	0.28872500	1.52297200	0.00004800
O	0.00586600	-0.70957100	0.00022300
C	0.74684200	0.37598300	0.00011900
C	2.22716600	0.11378100	0.00007800
C	2.74399800	-1.19071400	0.00004200
C	3.10187200	1.21069800	0.00002900
C	4.12538500	-1.39337100	-0.00005000
H	2.06151700	-2.03364100	0.00007600
C	4.48174000	1.00316600	-0.00005700
H	2.68535800	2.21267500	0.00005300
C	4.99565100	-0.29826500	-0.00010200
H	4.52232800	-2.40527800	-0.00008600
H	5.15598500	1.85577600	-0.00009700
H	6.07103800	-0.45820200	-0.00017800
Au	-1.99226400	-0.05830600	-0.00002900

Filename: AuCO2Ph
Sum of electronic and zero-point Energies = -15126.5532

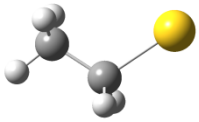
Figure S52: Cartesian coordinates and energies (eV) for [Au(O$_2$CR)]$^-$, R = Me, Et, Ph and CH$_2$Ph.



[Au(Me)]⁻

C	-1.82327700	0.00000100	0.00000100
H	-2.14876500	1.01927800	-0.21993700
H	-2.14873200	-0.70010900	-0.77276100
H	-2.14880200	-0.31918100	0.99266600
Au	0.22007500	0.00000000	0.00000000

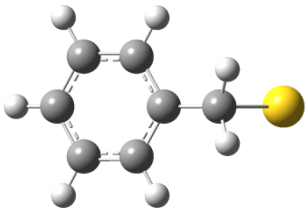
Filename: AuMe
Sum of electronic and zero-point Energies = -4779.7178



[Au(Et)]⁻

C	1.48318200	0.68808400	0.00000000
H	1.53147100	1.31885800	-0.89294900
H	1.53147100	1.31885600	0.89295000
C	2.54112900	-0.40791200	0.00000000
H	3.54018700	0.05740500	-0.00001100
H	2.47496000	-1.04622200	0.88651200
H	2.47494700	-1.04623800	-0.88650000
Au	-0.45188500	-0.02890700	0.00000000

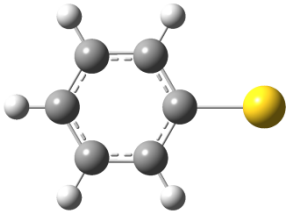
Filename: AuEt
Sum of electronic and zero-point Energies = -5848.7062



[Au(CH$_2$Ph)]⁻

C	-0.09904500	0.00034500	1.24135000
H	0.09802500	-0.89676800	1.83346600
H	0.09798900	0.89778200	1.83298700
C	-1.44124900	0.00015300	0.60298100
C	-2.10301900	-1.20802200	0.31194900
C	-2.10319400	1.20815900	0.31165000
C	-3.37911100	-1.20915400	-0.25150300
H	-1.60614900	-2.15142600	0.52777100
C	-3.37928900	1.20896500	-0.25179800
H	-1.60647000	2.15169100	0.52724400
C	-4.02320100	-0.00017700	-0.53763400
H	-3.87293900	-2.15351600	-0.46672700
H	-3.87325900	2.15319800	-0.46725700
H	-5.01720000	-0.00030500	-0.97729800
Au	1.45504600	-0.00002900	-0.14395100

Filename: AgCH2Ph
Sum of electronic and zero-point Energies = -11065.0114

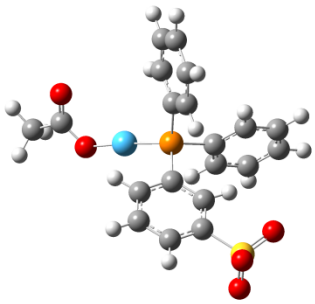


[Au(Ph)]⁻

C	-0.82535900	0.00000200	0.00016700
C	-1.52144800	1.21565200	0.00011300
C	-1.52144700	-1.21565000	0.00011500
C	-2.92219200	1.20832200	-0.00002700
H	-0.98964700	2.16141100	0.00019600
C	-2.92219100	-1.20832300	-0.00003200
H	-0.98964300	-2.16140900	0.00022000
C	-3.62426300	-0.00000100	-0.00011700
H	-3.45960500	2.15380200	-0.00004200
H	-3.45960300	-2.15380500	-0.00005500
H	-4.71128800	-0.00000100	-0.00023200
Au	1.18520500	0.00000000	-0.00001800

Filename: AuPh
Sum of electronic and zero-point Energies = -9995.7182

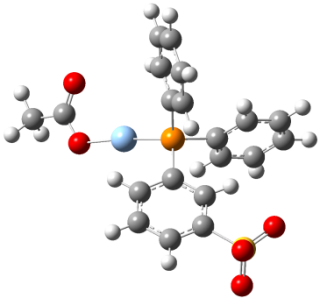
Figure S53: Cartesian coordinates and energies (eV) for [Au(R)]⁻, R = Me, Et, Ph and CH_2Ph.



$[(MeCO_2)Cu(PPh_2C_6H_4SO_3)]^-$

Cu	2.44705500	-0.96779000	0.23461800
P	0.66437500	0.29873500	0.05275100
C	0.90988500	1.75686300	-1.04419500
C	2.17271600	2.37466500	-1.03876400
C	-0.09935400	2.26610700	-1.87692800
C	2.41733800	3.49112700	-1.84254000
H	2.96780200	1.97943600	-0.41038200
C	0.15114800	3.37859000	-2.68711200
H	-1.08021200	1.79973800	-1.90094200
C	1.40699100	3.99410500	-2.66996900
H	3.39806300	3.96021800	-1.82914500
H	-0.63707000	3.76237900	-3.33034000
H	1.59974500	4.85754700	-3.30208700
C	0.08053700	0.97749500	1.66068100
C	-0.53165400	2.23549100	1.78012400
C	0.26359400	0.19070100	2.81118700
C	-0.95767400	2.69498300	3.03046500
H	-0.67955100	2.86124400	0.90462400
C	-0.17120000	0.64852900	4.05782400
H	0.75056400	-0.77895700	2.73308400
C	-0.78117400	1.90293600	4.16968800
H	-1.42913700	3.67137700	3.11168100
H	-0.02517600	0.03029700	4.94011800
H	-1.11324300	2.26286900	5.14042700
C	-0.78174500	-0.59680700	-0.66060300
C	-2.09001200	-0.43110800	-0.18280700
C	-0.54374200	-1.48433900	-1.72276500
C	-3.13630200	-1.14311200	-0.77400200
H	-2.30039100	0.24589300	0.63784500
C	-1.59970500	-2.18392800	-2.31195300
H	0.46875900	-1.63205400	-2.09118100
C	-2.90335900	-2.01928500	-1.83843900
H	-1.40582400	-2.86380500	-3.13730300
H	-3.72316900	-2.56629400	-2.29448600
S	-4.81766200	-0.97592200	-0.12786300
O	-4.82334900	0.26011600	0.71685200
O	-5.07514900	-2.22166100	0.66811400
O	-5.70891800	-0.86977400	-1.32845500
O	5.37253000	-0.96901900	-0.74729100
O	3.94320600	-2.14384600	0.53537900
C	5.10161300	-1.93884900	0.00014000
C	6.16431600	-2.96950500	0.34137700
H	7.10708000	-2.75243900	-0.16707600
H	6.33391200	-2.98152000	1.42508300
H	5.82039600	-3.97079000	0.05544900

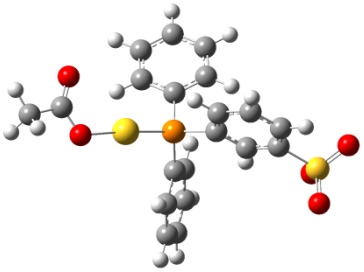
Filename: Methanol_CuCO2MePPh3SO3
Sum of electronic and zero-point Energies = -56745.9390



$[(MeCO_2)Ag(PPh_2C_6H_4SO_3)]^-$

P	0.39404500	0.39701300	0.01337400
C	0.51222600	1.90335900	-1.03510300
C	1.72437600	2.61531500	-1.02707100
C	-0.54916500	2.36111800	-1.83185100
C	1.86615200	3.77652400	-1.79071000
H	2.55939500	2.26039700	-0.42694900
C	-0.40020400	3.51898600	-2.60277000
H	-1.49154600	1.82167900	-1.85767900
C	0.80391400	4.22979800	-2.58134600
H	2.80777700	4.31970100	-1.77497500
H	-1.22755600	3.86344900	-3.21838200
H	0.91694400	5.12906900	-3.18186800
C	-0.15345100	0.97625100	1.67069700
C	-0.82311300	2.19531600	1.86359700
C	0.11487200	0.15531400	2.77974600
C	-1.22381600	2.58145300	3.14672600
H	-1.03518500	2.84636100	1.02048000
C	-0.29515200	0.53982600	4.05883700
H	0.64827800	-0.78328600	2.64495300
C	-0.96418200	1.75474800	4.24449300
H	-1.74083400	3.52779800	3.28543800
H	-0.08362300	-0.10407800	4.90890700
H	-1.27650000	2.05795600	5.24080700
C	-1.01663000	-0.56954900	-0.67086900
C	-2.32174900	-0.45418700	-0.16759500
C	-0.76164800	-1.45098200	-1.73287200
C	-3.34769000	-1.21205100	-0.73451500
H	-2.54393900	0.21701600	0.65450200
C	-1.79928500	-2.19761000	-2.29781700
H	0.24905300	-1.55855000	-2.11963600
C	-3.09836200	-2.08434500	-1.79943800
H	-1.59274000	-2.87510200	-3.12197600
H	-3.90261000	-2.67013800	-2.23521200
S	-5.03287800	-1.08915000	-0.08803400
O	-5.01582800	0.00064200	0.93619200
O	-5.34525600	-2.43501500	0.49677000
O	-5.89686100	-0.76792600	-1.27052700
O	5.50679200	-0.34288900	-0.16953300
O	4.16915100	-2.12740600	0.12360000
C	5.32741900	-1.57579900	-0.01930900
C	6.51006500	-2.52985600	0.00235100
H	7.45551600	-1.99433300	-0.11578000
H	6.52387100	-3.08411100	0.94842100
H	6.40830300	-3.26611000	-0.80411300
Ag	2.42487900	-0.85228800	0.07612500

Filename: Methanol_AgCO2MePPh3SO3_2
Sum of electronic and zero-point Energies = -55375.4082

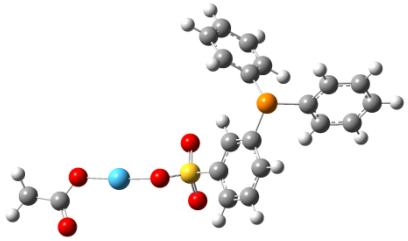


$[(MeCO_2)Au(PPh_2C_6H_4SO_3)]^-$

P	0.13781000	0.48198100	0.02034000
C	0.21373600	1.87132800	-1.17731500
C	1.39715000	2.62664400	-1.24844700
C	-0.86824900	2.20349200	-2.00798900
C	1.49033800	3.70744800	-2.12844100
H	2.24656300	2.36638400	-0.62157700
C	-0.76731300	3.28172600	-2.89298100
H	-1.78902300	1.62903100	-1.97352000
C	0.40870900	4.03560800	-2.95354800
H	2.41018700	4.28479600	-2.17584700
H	-1.60967800	3.52930100	-3.53407500
H	0.48458500	4.87164200	-3.64442800
C	-0.46602000	1.18157200	1.60734100
C	-1.06382300	2.44821000	1.68857600
C	-0.32242100	0.40794400	2.77261000
C	-1.51555700	2.93245000	2.92112900
H	-1.18127200	3.06094300	0.79982300
C	-0.78278900	0.89183100	3.99873000
H	0.15110000	-0.56973700	2.72335400
C	-1.37825200	2.15654700	4.07565500
H	-1.97531700	3.91612500	2.97448500
H	-0.66863500	0.28533700	4.89366000
H	-1.73009000	2.53531500	5.03206600
C	-1.18842000	-0.64334100	-0.57424700
C	-2.52643300	-0.46877400	-0.18986100
C	-0.84778500	-1.68741500	-1.44844500
C	-3.50365700	-1.33048300	-0.69209800
H	-2.81098700	0.33000300	0.48679800
C	-1.83612800	-2.54033100	-1.94551500
H	0.18930200	-1.83657200	-1.73795200
C	-3.16983300	-2.36727700	-1.56887900
H	-1.56556200	-3.34536500	-2.62335500
H	-3.93750300	-3.03113100	-1.95500500
S	-5.22243200	-1.14074600	-0.15944600
O	-5.35740000	0.27225000	0.31678300
O	-5.42483300	-2.14219200	0.93899400
O	-6.05919900	-1.43551400	-1.36624500
O	4.90669700	-0.87020700	-1.34013000
O	4.00273600	-1.53711200	0.61541600
C	4.97522900	-1.46373000	-0.24393600
C	6.24708100	-2.16961700	0.18777900
H	7.00748000	-2.12212100	-0.59546500
H	6.63770800	-1.70209200	1.09983000
H	6.03191100	-3.21795200	0.42487100
Au	2.15295700	-0.56585400	0.25662200

Filename: Methanol_AuCO2MePPh3SO3
Sum of electronic and zero-point Energies = -55069.9152

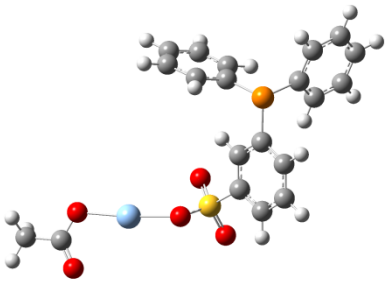
Figure S54: Cartesian coordinates and energies (eV) for $[(MeCO_2)M(PPh_2C_6H_4SO_3)]^-$ in methanol bound through P.



[(MeCO$_2$)Cu(O$_3$SC$_6$H$_4$PPh$_2$)]$^-$

Cu	4.45017000	0.08097700	-0.09173800
P	-3.36735300	0.20512900	-1.37174500
C	-1.96691400	-0.92407100	-0.91658200
C	-0.83218600	-0.50713000	-0.20441000
C	-2.01328200	-2.24608000	-1.39666800
C	0.21341100	-1.40672300	0.02139500
H	-0.75647800	0.50551200	0.17568600
C	-0.96920800	-3.13981900	-1.14796600
H	-2.87535200	-2.58498700	-1.96746700
C	0.15972400	-2.72532000	-0.43672700
H	-1.02924600	-4.16057500	-1.51631500
H	0.97721200	-3.41470100	-0.24893400
S	1.69095600	-0.84713100	0.88271100
O	1.36755600	0.43784200	1.55927500
O	2.69360600	-0.65542200	-0.26104400
O	2.11565800	-1.93854900	1.80319600
O	7.28726100	-0.94863000	-0.57280200
O	6.15450400	0.90854100	0.01531700
C	7.24411300	0.25819600	-0.23817600
C	8.52414000	1.05982600	-0.08125800
H	9.37985000	0.52283400	-0.49849500
H	8.42999400	2.03794100	-0.56545000
H	8.70754400	1.23966400	0.98613000
C	-4.76306500	-0.44004000	-0.33656300
C	-6.06498900	-0.09141200	-0.74074300
C	-4.60560200	-1.25959000	0.79420400
C	-7.18055300	-0.53481300	-0.02365800
H	-6.20980400	0.52812400	-1.62383400
C	-5.72209700	-1.71347500	1.50483600
H	-3.61261500	-1.54935800	1.12640700
C	-7.01132300	-1.35025600	1.10075800
H	-8.17896100	-0.25248700	-0.34956300
H	-5.58202300	-2.34786600	2.37713800
H	-7.87758500	-1.70465000	1.65436400
C	-2.91704900	1.79595100	-0.53535900
C	-2.28759700	2.77657400	-1.32306000
C	-3.18337500	2.08283600	0.81443600
C	-1.91620200	4.00718100	-0.77136700
H	-2.08528000	2.57864100	-2.37377800
C	-2.82199800	3.31717100	1.36375600
H	-3.67141900	1.34408700	1.44414200
C	-2.18554700	4.28108700	0.57360900
H	-1.42574600	4.75200500	-1.39371000
H	-3.03637500	3.52390100	2.40982200
H	-1.90471500	5.23994600	1.00277500

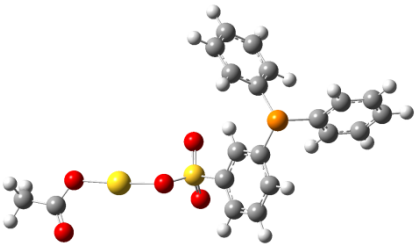
Filename: Methanol_CuCO2MeSO3PPh3
Sum of electronic and zero-point Energies = -56745.4324



[(MeCO$_2$)Ag(O$_3$SC$_6$H$_4$PPh$_2$)]$^-$

P	-3.64709800	0.40778300	-1.34853400
C	-2.43956400	-0.97172800	-1.06145400
C	-1.24366900	-0.83179500	-0.34247900
C	-2.73141500	-2.21576200	-1.65091400
C	-0.37784900	-1.92272600	-0.21789800
H	-0.98726700	0.11236500	0.12604200
C	-1.86505400	-3.30147800	-1.50683600
H	-3.64702700	-2.34031800	-2.22546500
C	-0.67342700	-3.16214500	-0.78958500
H	-2.11221500	-4.25754900	-1.96088700
H	0.00680300	-4.00085300	-0.67984600
S	1.18106100	-1.70743300	0.65771800
O	0.99989700	-0.59757600	1.63426700
O	2.17098100	-1.32827400	-0.44368900
O	1.52852800	-3.01945600	1.27194200
O	6.97340700	-0.34742600	-0.19145800
O	5.53844200	1.32929700	0.24117800
C	6.72802100	0.84082800	0.12742900
C	7.86276100	1.80535400	0.43108200
H	8.83019400	1.37575400	0.15886200
H	7.71664700	2.75117100	-0.10212100
H	7.86470800	2.03196500	1.50496600
C	-4.97376100	0.04950600	-0.10475200
C	-6.21297900	0.68817800	-0.29706800
C	-4.83155300	-0.83164200	0.98024100
C	-7.27661700	0.46726700	0.58291600
H	-6.34951000	1.36109000	-1.14160000
C	-5.90011500	-1.06293300	1.85391100
H	-3.88793600	-1.34218100	1.15105700
C	-7.12319600	-0.41240300	1.66055900
H	-8.22557800	0.97302100	0.42010200
H	-5.77310600	-1.74929100	2.68806100
H	-7.95220400	-0.59357800	2.34056900
C	-2.78086000	1.88214300	-0.63648700
C	-2.01143700	2.65845000	-1.52245500
C	-2.87038300	2.28204900	0.70758200
C	-1.33160700	3.79448900	-1.07259500
H	-1.94307300	2.37491200	-2.57099900
C	-2.19995400	3.42546300	1.15543700
H	-3.46185100	1.70340300	1.41175900
C	-1.42690200	4.18236300	0.26838900
H	-0.73732400	4.37978700	-1.77038600
H	-2.27974300	3.72151600	2.19894200
H	-0.90595300	5.07032400	0.61855600
Ag	3.91577100	-0.06048400	-0.08406700

Filename: Methanol_AgCO2MeSO3PPh3
Sum of electronic and zero-point Energies = -55374.7850

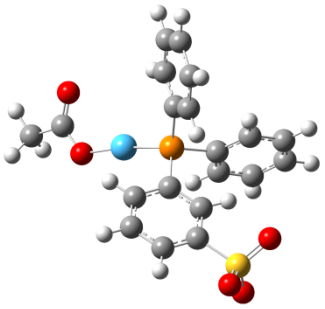


[(MeCO$_2$)Au(O$_3$SC$_6$H$_4$PPh$_2$)]$^-$

P	-4.28019500	0.18771500	-1.36774200
C	-2.84571300	-0.92141600	-0.97376400
C	-1.70753400	-0.50449900	-0.26773800
C	-2.88006000	-2.23203600	-1.48463700
C	-0.64875400	-1.39663000	-0.07827700
H	-1.64134500	0.49913000	0.13726100
C	-1.82045500	-3.11724200	-1.27321000
H	-3.74585100	-2.56902900	-2.05091700
C	-0.68793800	-2.70458500	-0.56728100
H	-1.87146900	-4.12925300	-1.66590800
H	0.14126700	-3.38635600	-0.40537000
S	0.82092900	-0.84516200	0.79599800
O	0.50143400	0.42370800	1.49693900
O	1.81199500	-0.61715300	-0.37280000
O	1.27492400	-1.95142200	1.67813700
O	6.67622000	-0.96770900	-0.61605700
O	5.65616000	0.85239700	0.24702800
C	6.70848300	0.16884100	-0.10879700
C	8.01794000	0.89506700	0.13092900
H	8.86778600	0.23739400	-0.06623400
H	8.07731800	1.76654300	-0.53284100
H	8.06742000	1.26362100	1.16145800
C	-5.61007000	-0.46407700	-0.25347700
C	-6.93558900	-0.12899200	-0.58601700
C	-5.38202400	-1.27679700	0.87008300
C	-8.00502600	-0.57909400	0.19416800
H	-7.13504800	0.48541700	-1.46199400
C	-6.45293500	-1.73808400	1.64352100
H	-4.36896500	-1.55415200	1.14812400
C	-7.76595900	-1.38850500	1.31030300
H	-9.02263800	-0.30737000	-0.07666100
H	-6.25861200	-2.36727900	2.50917700
H	-8.59674900	-1.74821700	1.91270500
C	-3.80577100	1.79215900	-0.57235900
C	-3.19668000	2.75762000	-1.39447100
C	-4.04040100	2.10583600	0.77724400
C	-2.81399600	3.99917200	-0.87659000
H	-3.01983300	2.53953400	-2.44587300
C	-3.66768600	3.35150100	1.29293500
H	-4.51353500	1.38001000	1.43282000
C	-3.05153000	4.29979100	0.46884300
H	-2.34005800	4.73194700	-1.52544700
H	-3.85739600	3.57885600	2.33948000
H	-2.76187200	5.26741900	0.87166600
Au	3.76243000	0.07078300	-0.03133800

Filename: Methanol_AuCO2MeSO3PPh3_2
Sum of electronic and zero-point Energies = -55068.7183

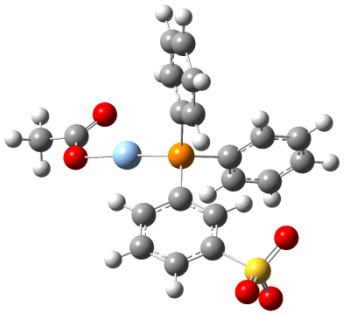
Figure S55: Cartesian coordinates and energies (eV) for [(MeCO$_2$)M(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$ in methanol bound through O.



[(MeCO$_2$)Cu(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

Cu	2.46337600	-0.94043300	0.10391300
P	0.67460700	0.33355800	0.03780900
C	0.85901900	1.85873300	-0.97560900
C	2.10968300	2.50038400	-0.97701600
C	-0.19074900	2.39882400	-1.73582900
C	2.30205600	3.67151700	-1.71493500
H	2.93452500	2.08201200	-0.40523600
C	0.00731200	3.56612900	-2.48040100
H	-1.16215800	1.91365600	-1.75352900
C	1.25103900	4.20601500	-2.46867700
H	3.27288200	4.15985900	-1.70732900
H	-0.81162400	3.97395600	-3.06717500
H	1.40255600	5.11260600	-3.04862600
C	0.09179400	0.90113200	1.68868800
C	-0.57697700	2.12052400	1.88290200
C	0.32881200	0.06386300	2.79265800
C	-1.00696700	2.49129200	3.16092700
H	-0.76447700	2.78409000	1.04401500
C	-0.10964100	0.43294700	4.06726200
H	0.85999300	-0.87526600	2.65627100
C	-0.77748600	1.64836100	4.25343100
H	-1.52203000	3.43815900	3.30050000
H	0.07777900	-0.22354000	4.91283400
H	-1.11261300	1.93939900	5.24553700
C	-0.76126800	-0.55469900	-0.70705700
C	-2.06618000	-0.43723900	-0.21259200
C	-0.51592600	-1.38894800	-1.81178900
C	-3.10541300	-1.14475400	-0.82606000
H	-2.27705500	0.20104500	0.63878900
C	-1.56189000	-2.08397700	-2.42020400
H	0.49567600	-1.49802800	-2.19451600
C	-2.86562700	-1.96913400	-1.92704700
H	-1.36274900	-2.72328200	-3.27559100
H	-3.67944000	-2.51261800	-2.39534500
S	-4.77017600	-1.02806700	-0.13001700
O	-4.93694700	0.39586000	0.30821200
O	-4.80163000	-1.98684500	1.02546500
O	-5.71335900	-1.41725600	-1.22646500
O	5.51860900	-0.79348000	-0.32878700
O	3.87916100	-2.25078100	0.18695700
C	5.11922200	-1.94329700	-0.01843200
C	6.10641600	-3.08585700	0.14079900
H	7.12782600	-2.76091700	-0.07004300
H	6.05615600	-3.47633000	1.16413100
H	5.84048500	-3.90741600	-0.53419700

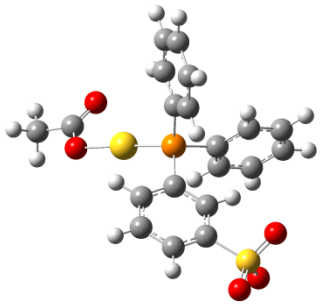
Filename: Water_CuCO2MePPh3SO3_3
Sum of electronic and zero-point Energies = -56745.8750



[(MeCO$_2$)Ag(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

P	0.39183300	0.40209200	-0.04717900
C	0.35610900	2.03159200	-0.89826900
C	1.52597400	2.81071900	-0.86954500
C	-0.77856800	2.51874000	-1.56546600
C	1.55403900	4.06521000	-1.48320800
H	2.41620200	2.43591400	-0.36975400
C	-0.74322700	3.77083300	-2.18880100
H	-1.69020700	1.93037100	-1.60406000
C	0.41926800	4.54651400	-2.14651800
H	2.46317900	4.65977800	-1.45208700
H	-1.62630700	4.13741500	-2.70554200
H	0.44385700	5.51846200	-2.63210500
C	-0.03802600	0.74759200	1.70678500
C	-0.68368700	1.92738300	2.10916800
C	0.30308500	-0.21557700	2.67206600
C	-0.98871600	2.13546100	3.45848400
H	-0.94950300	2.68524900	1.37825900
C	-0.01216900	-0.00882900	4.01711400
H	0.81903800	-1.12512200	2.37323000
C	-0.65652900	1.16890000	4.41305000
H	-1.48709200	3.05278300	3.76081300
H	0.25467200	-0.76106300	4.75459500
H	-0.89323500	1.33417000	5.46081000
C	-1.03152400	-0.54907000	-0.72666100
C	-2.32210200	-0.45092800	-0.18849600
C	-0.80334800	-1.39864600	-1.82205500
C	-3.36429000	-1.19188800	-0.75307800
H	-2.51884800	0.19922300	0.65739600
C	-1.85362400	-2.12966600	-2.38058300
H	0.19802300	-1.49277800	-2.23463500
C	-3.14152300	-2.03296800	-1.84619000
H	-1.66852800	-2.78253700	-3.22873800
H	-3.95783700	-2.60375400	-2.27621500
S	-5.00947300	-1.09925600	-0.00765500
O	-5.17656100	0.31765400	0.45169200
O	-4.99992900	-2.07282900	1.13534400
O	-5.97840200	-1.48435300	-1.08292400
O	5.33581000	-0.62456700	0.89810500
O	4.29297600	-1.86587100	-0.66343700
C	5.32638500	-1.54588400	0.04271000
C	6.57153000	-2.38310200	-0.19281400
H	7.45206500	-1.91697800	0.25580200
H	6.42712200	-3.37118900	0.26234100
H	6.73935000	-2.53711700	-1.26359400
Ag	2.47290700	-0.74180200	-0.30559100

Filename: Water_AgCO2MePPh3SO3_2
Sum of electronic and zero-point Energies = -55375.3450

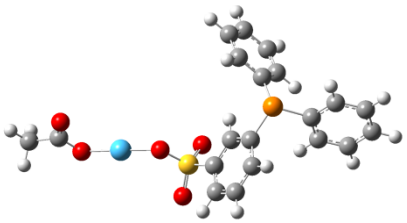


[(MeCO$_2$)Au(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$

P	0.14193600	0.51936100	-0.00413800
C	0.20911800	2.19871700	-0.74141700
C	1.40539800	2.92895300	-0.63668800
C	-0.89715300	2.77161600	-1.38823600
C	1.48826400	4.22057600	-1.16176200
H	2.27162700	2.48716500	-0.15094100
C	-0.80635400	4.06192300	-1.92027300
H	-1.82784300	2.22007700	-1.48051000
C	0.38317000	4.78804800	-1.80661900
H	2.41708800	4.77796300	-1.07580900
H	-1.66667900	4.49646600	-2.42221000
H	0.45100700	5.79012900	-2.22174800
C	-0.32209700	0.73856500	1.75665100
C	-0.98767900	1.88782900	2.21180400
C	-0.00430900	-0.28404600	2.66660900
C	-1.33371600	2.00798600	3.56136900
H	-1.23704700	2.68932800	1.52309300
C	-0.35978900	-0.16328300	4.01196700
H	0.52484100	-1.16983400	2.32483500
C	-1.02287900	0.98404700	4.46176900
H	-1.84593200	2.90228100	3.90602300
H	-0.11069500	-0.95984000	4.70782400
H	-1.29124000	1.08123100	5.51039500
C	-1.27496000	-0.32736500	-0.81414100
C	-2.52900400	-0.42127000	-0.20101500
C	-1.08195300	-0.88589600	-2.09037100
C	-3.57591600	-1.06837600	-0.86783600
H	-2.69461100	0.00302900	0.78382600
C	-2.13563900	-1.52021500	-2.74653000
H	-0.10745700	-0.82642700	-2.56763900
C	-3.39149700	-1.61834300	-2.13612100
H	-1.98088000	-1.94766500	-3.73302300
H	-4.21094800	-2.11759800	-2.64150900
S	-5.17774600	-1.19158800	-0.03804400
O	-5.55950300	0.21186800	0.32840000
O	-4.94848700	-2.05163500	1.17000300
O	-6.11843800	-1.81211800	-1.02319100
O	5.04894900	-0.58524600	0.93904800
O	3.86324600	-1.78041600	-0.56371900
C	4.94775400	-1.50870700	0.10176100
C	6.11908900	-2.42263400	-0.20258300
H	7.01632900	-2.10119600	0.33075300
H	5.87057900	-3.44825600	0.09493000
H	6.31813500	-2.43498500	-1.27987600
Au	2.09561300	-0.63588900	-0.25432900

Filename: Water_AuCO2MePPh3SO3
Sum of electronic and zero-point Energies = -55069.8419

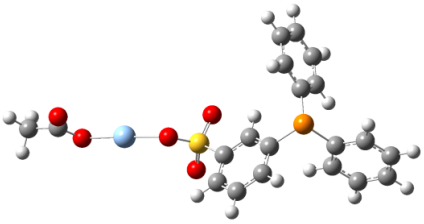
Figure S56: Cartesian coordinates and energies (eV) for [(MeCO$_2$)M(PPh$_2$C$_6$H$_4$SO$_3$)]$^-$ in water bound through P.



$[(MeCO_2)Cu(O_3SC_6H_4PPh_2)]^-$

Cu	4.38395300	-0.19017200	0.16251300
P	-3.28675200	0.39712200	-1.39273400
C	-1.95966900	-0.85277600	-1.04312800
C	-0.84250900	-0.60426000	-0.23464400
C	-2.06365900	-2.10080100	-1.68646100
C	0.13500900	-1.59349400	-0.08006300
H	-0.73164100	0.34702100	0.27438900
C	-1.09002300	-3.08468100	-1.51052100
H	-2.91666000	-2.30767500	-2.32877400
C	0.02597700	-2.83662800	-0.70529900
H	-1.19376100	-4.04581800	-2.00620300
H	0.79007500	-3.59478900	-0.57144400
S	1.59459400	-1.23055600	0.90795700
O	1.17756500	-0.33383000	2.02236800
O	2.50758300	-0.49984800	-0.08423600
O	2.17752700	-2.52815300	1.34780000
O	6.49098000	1.28787600	-1.48043200
O	6.25194300	0.07064000	0.40296000
C	6.95766500	0.74296200	-0.45040200
C	8.43600700	0.84672300	-0.12254400
H	8.98366900	1.35213000	-0.92123100
H	8.56553900	1.40723800	0.81114200
H	8.85849300	-0.15189600	0.03509500
C	-4.69420300	-0.23342500	-0.36520200
C	-5.98817300	0.17649300	-0.73404300
C	-4.54854800	-1.10342600	0.72906400
C	-7.10835700	-0.25925200	-0.01898800
H	-6.12327700	0.83693400	-1.58792500
C	-5.66936800	-1.54703500	1.43889900
H	-3.56098500	-1.43965600	1.03189600
C	-6.95097000	-1.12440600	1.06926000
H	-8.10064000	0.06901500	-0.31793300
H	-5.53942200	-2.22029200	2.28264000
H	-7.82071800	-1.47130000	1.62129700
C	-2.70863200	1.89030800	-0.46130000
C	-1.95640100	2.83851100	-1.17837900
C	-2.99621200	2.14038400	0.89097500
C	-1.48868300	3.99974000	-0.55526600
H	-1.73467500	2.67025000	-2.23013000
C	-2.53834600	3.30746000	1.51180600
H	-3.57746800	1.42604400	1.46658200
C	-1.78186700	4.23846200	0.79178000
H	-0.90541500	4.71968500	-1.12373800
H	-2.77141600	3.48647900	2.55854800
H	-1.42755200	5.14502200	1.27564000

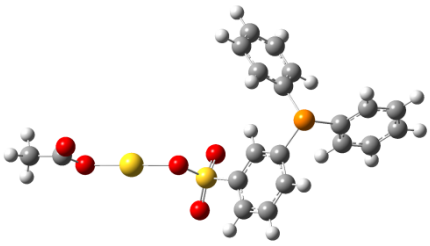
Filename: Water_CuCO2MeSO3PPh3
Sum of electronic and zero-point Energies = -56745.3451



$[(MeCO_2)Ag(O_3SC_6H_4PPh_2)]^-$

P	4.02398200	0.13561800	1.37161500
C	2.42952900	-0.78616700	1.14146300
C	1.34365100	-0.29898600	0.39721000
C	2.29840700	-2.02195200	1.79820600
C	0.16845700	-1.04889300	0.31750500
H	1.40895500	0.65103800	-0.12051100
C	1.12148200	-2.76941200	1.69867400
H	3.12317100	-2.40809600	2.39297900
C	0.04155400	-2.28530100	0.95817700
H	1.04072000	-3.72541000	2.20826200
H	-0.87714500	-2.85931700	0.88736700
S	-1.22590900	-0.42442300	-0.63539500
O	-0.80913900	0.86288000	-1.25738400
O	-2.32127300	-0.22297700	0.41073600
O	-1.60385300	-1.48191600	-1.61910100
O	-7.05630700	0.66615700	1.30116000
O	-6.51583200	-0.09803200	-0.74606800
C	-7.36722100	0.30731500	0.13789500
C	-8.81796200	0.32017100	-0.31293700
H	-9.46980500	0.74024300	0.45641800
H	-8.91872900	0.90326100	-1.23500200
H	-9.14030300	-0.70365200	-0.53681300
C	5.14969800	-0.70699600	0.16490800
C	6.53292300	-0.54167500	0.36228200
C	4.71232500	-1.50461100	-0.90617800
C	7.45588400	-1.14008100	-0.50105200
H	6.89269500	0.05729100	1.19633100
C	5.63574300	-2.11318000	-1.76328200
H	3.65045200	-1.65497200	-1.07870000
C	7.00853500	-1.92958400	-1.56607600
H	8.52076200	-0.99772100	-0.33505300
H	5.28050700	-2.72713200	-2.58726900
H	7.72417100	-2.40241300	-2.23376400
C	3.67846300	1.76509800	0.56069500
C	3.12915800	2.77735000	1.36923900
C	3.95724400	2.05481200	-0.78541000
C	2.84444900	4.03981300	0.84053500
H	2.92099500	2.57923300	2.41866800
C	3.68521400	3.32275000	-1.31140700
H	4.38662700	1.29379100	-1.43061300
C	3.12516600	4.31679600	-0.50223900
H	2.41419200	4.80736300	1.47888100
H	3.90883200	3.53027300	-2.35497700
H	2.91372700	5.30069900	-0.91299700
Ag	-4.44404200	-0.12724400	-0.12606600

Filename: Water_AgCO2MeSO3PPh3
Sum of electronic and zero-point Energies = -55374.6852

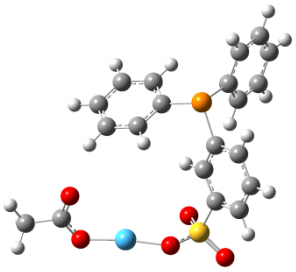


$[(MeCO_2)Au(O_3SC_6H_4PPh_2)]^-$

P	4.21364900	0.39868100	1.38502300
C	2.84762900	-0.84209900	1.18493400
C	1.72415000	-0.64921800	0.36917600
C	2.94048600	-2.02619500	1.93935500
C	0.72951900	-1.63114600	0.32200400
H	1.62447300	0.25121600	-0.22739800
C	1.94536000	-3.00340300	1.87306900
H	3.79907800	-2.18553700	2.58758300
C	0.82216900	-2.81057400	1.06404000
H	2.03732700	-3.91347800	2.45892900
H	0.04109000	-3.56169900	1.01473200
S	-0.72513400	-1.34708300	-0.69418800
O	-0.31477200	-0.55883200	-1.88542900
O	-1.61401700	-0.50310500	0.25345800
O	-1.34347600	-2.66325100	-0.99784900
O	-5.96010900	1.32076100	1.39622200
O	-5.62909600	0.21913600	-0.54915400
C	-6.36641100	0.87837600	0.30348100
C	-7.79232000	1.10199800	-0.15934700
H	-8.43365800	1.37209000	0.68266400
H	-7.80173300	1.92512100	-0.88510400
H	-8.18706900	0.21342400	-0.66057800
C	5.48092800	-0.20164700	0.17513300
C	6.79882200	0.25676500	0.35458100
C	5.21297000	-1.08897500	-0.88081500
C	7.81985300	-0.14378900	-0.51252300
H	7.03027100	0.93104100	1.17649300
C	6.23699800	-1.50012300	-1.74100000
H	4.20515700	-1.46194400	-1.03909300
C	7.54105100	-1.02613100	-1.56224900
H	8.83155100	0.22427000	-0.36172500
H	6.01313400	-2.18768400	-2.55288500
H	8.33486700	-1.34644900	-2.23211600
C	3.52113200	1.90812500	0.56400200
C	2.72999100	2.75976000	1.35776100
C	3.77043900	2.26979800	-0.77005100
C	2.18332300	3.93069300	0.82546300
H	2.53851400	2.50670500	2.39856800
C	3.23489300	3.44973700	-1.29927200
H	4.38282100	1.63467700	-1.40335200
C	2.43763500	4.28057700	-0.50574000
H	1.56938600	4.57269100	1.45210000
H	3.43943700	3.71547800	-2.33345800
H	2.02178100	5.19586100	-0.91892100
Au	-3.63378400	-0.13045000	-0.15158000

Filename: Water_AuCO2MeSO3PPh3
Sum of electronic and zero-point Energies = -55068.6199

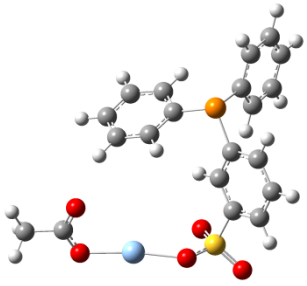
Figure S57: Cartesian coordinates and energies (eV) for $[(MeCO_2)M(PPh_2C_6H_4SO_3)]^-$ in water bound through O.



$[(MeCO_2)Cu(O_3SC_6H_4PPh_2)]^-$

Cu	-3.60608900	-0.55580400	-0.23880300
P	2.65245900	0.68376200	1.39986800
C	1.68714400	-0.89453200	1.25852900
C	0.66325700	-1.12968900	0.32657200
C	2.01523900	-1.91268000	2.17091700
C	-0.00719300	-2.35426300	0.31579200
H	0.37373200	-0.36985600	-0.39206000
C	1.35530600	-3.14416300	2.13807400
H	2.79225700	-1.73656700	2.91225300
C	0.33553400	-3.36996300	1.21070500
H	1.62768000	-3.92429700	2.84562700
H	-0.19437300	-4.31636700	1.16984200
S	-1.38045800	-2.61086800	-0.84142800
O	-1.10540000	-1.75760400	-2.01666600
O	-2.59196800	-2.12399500	-0.02884600
O	-1.46008600	-4.06956900	-1.06084300
O	-3.78929800	2.26308400	1.04220100
O	-4.79962600	0.85871000	-0.42136700
C	-4.68244000	1.97212300	0.23290100
C	-5.79724800	2.97489100	-0.08142100
H	-5.65988300	3.89629500	0.49063700
H	-5.80123100	3.20317400	-1.15411800
H	-6.77284800	2.53464400	0.15777400
C	3.99118800	0.44196800	0.12808900
C	5.27099300	0.93208900	0.43438900
C	3.79836700	-0.20521200	-1.10459800
C	6.33083400	0.79338300	-0.46927300
H	5.43756500	1.42439700	1.39035500
C	4.85566900	-0.35153400	-2.00560500
H	2.81970000	-0.59955600	-1.36298300
C	6.12460200	0.14920700	-1.69177200
H	7.31435500	1.18253300	-0.21460400
H	4.68692800	-0.85677000	-2.95379400
H	6.94637900	0.03381200	-2.39505800
C	1.55313700	1.92996300	0.58221000
C	0.21668600	2.04929400	1.00650900
C	2.03965800	2.85077300	-0.36083000
C	-0.62463400	3.03258100	0.48065900
H	-0.19254300	1.35026500	1.73173600
C	1.20709200	3.85266200	-0.87092800
H	3.06577900	2.78268700	-0.71143900
C	-0.12484000	3.94205800	-0.45809300
H	-1.66867600	3.05477200	0.78418000
H	1.60033100	4.55146500	-1.60686700
H	-0.77720200	4.70639700	-0.87414800

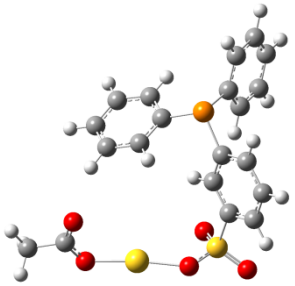
Filename: CuCO2MeSO3PPh3_2
Sum of electronic and zero-point Energies = -56742.5792



$[(MeCO_2)Ag(O_3SC_6H_4PPh_2)]^-$

P	2.92616600	0.73087700	1.39688400
C	2.04278800	-0.89327900	1.23876800
C	0.99700500	-1.15230600	0.33842100
C	2.45475800	-1.91934200	2.10754200
C	0.38264200	-2.40638000	0.31730000
H	0.64849500	-0.38854600	-0.34909700
C	1.85374400	-3.17999400	2.06148500
H	3.25051200	-1.72666400	2.82457600
C	0.80859100	-3.42828200	1.16818500
H	2.19095000	-3.96609000	2.73370300
H	0.32198200	-4.39741400	1.12054700
S	-1.03340800	-2.68916000	-0.78267800
O	-0.84079400	-1.79635300	-1.94821200
O	-2.21919900	-2.25750300	0.08624800
O	-1.06174200	-4.14458500	-1.04177100
O	-3.66583100	2.28388300	1.07316500
O	-4.80774900	1.07914400	-0.46058100
C	-4.59828300	2.12666900	0.26574800
C	-5.63266100	3.23889800	0.05919800
H	-5.42198600	4.08965100	0.71271800
H	-5.62030700	3.56682900	-0.98727900
H	-6.63897700	2.85521100	0.26518700
C	4.27595400	0.56984200	0.12562500
C	5.51252200	1.17012200	0.41403500
C	4.13341100	-0.12094900	-1.09011900
C	6.57704500	1.09756400	-0.49149000
H	5.64178600	1.69647500	1.35761000
C	5.19648400	-0.20116500	-1.99293600
H	3.18927800	-0.60000500	-1.33387600
C	6.42057900	0.40989300	-1.69780900
H	7.52627800	1.57146700	-0.25074000
H	5.06697200	-0.74105200	-2.92813200
H	7.24688200	0.34563000	-2.40230600
C	1.76290700	1.92529000	0.58977000
C	0.44357600	2.01728300	1.07210600
C	2.17491900	2.82624800	-0.40557400
C	-0.45435100	2.95147400	0.55087600
H	0.09504900	1.33204000	1.84141400
C	1.28626900	3.78170600	-0.91109900
H	3.18599200	2.77862800	-0.79984400
C	-0.02798800	3.84167700	-0.44163700
H	-1.48581500	2.95603900	0.89592500
H	1.62196100	4.46609300	-1.68786500
H	-0.72499500	4.56765500	-0.85371500
Ag	-3.41168000	-0.50189500	-0.21128500

Filename: AgCO2MeSO3PPh3_6
Sum of electronic and zero-point Energies = -55372.1081



$[(MeCO_2)Au(O_3SC_6H_4PPh_2)]^-$

P	3.29856500	0.71727100	1.39309300
C	2.30876600	-0.85015700	1.31569300
C	1.28394000	-1.11215100	0.39055700
C	2.62451600	-1.83330100	2.26929700
C	0.60867200	-2.33366800	0.42270200
H	1.00231900	-0.37714500	-0.35665500
C	1.95267600	-3.05884100	2.28558100
H	3.40202800	-1.63430300	3.00416200
C	0.93812400	-3.31455000	1.36134300
H	2.21460700	-3.81154400	3.02590500
H	0.40438400	-4.25956100	1.35363400
S	-0.73732500	-2.65231900	-0.75093000
O	-0.46571300	-1.82098200	-1.93930900
O	-1.99646700	-2.19703600	0.02754100
O	-0.78012100	-4.11734200	-0.92600200
O	-3.16914900	2.50162400	1.24299100
O	-4.12739600	1.30721700	-0.43530300
C	-3.98822800	2.35161400	0.33155900
C	-4.99367100	3.45393900	-0.01321400
H	-4.82808400	4.32983300	0.61922900
H	-4.89854800	3.73369300	-1.06879500
H	-6.01530400	3.08342900	0.13310400
C	4.59185900	0.44277500	0.08180600
C	5.87820300	0.94910300	0.32980100
C	4.36091000	-0.23763500	-1.12597500
C	6.90632200	0.79478200	-0.60718600
H	6.07479600	1.46718300	1.26626900
C	5.38711300	-0.40046500	-2.05971400
H	3.37707600	-0.64485700	-1.34026000
C	6.66211400	0.11754700	-1.80463200
H	7.89497100	1.19767300	-0.39777100
H	5.18871400	-0.93141900	-2.98786300
H	7.45925100	-0.00989300	-2.53371000
C	2.18641300	1.96355200	0.59431400
C	0.86919600	2.10700900	1.06767100
C	2.65030600	2.86639000	-0.37701900
C	0.02534300	3.10076300	0.56672700
H	0.47760500	1.42082100	1.81459500
C	1.81438800	3.87616200	-0.86549000
H	3.66125600	2.77883800	-0.76528400
C	0.50204000	3.99274500	-0.40021800
H	-1.00376800	3.14806100	0.91414100
H	2.18915300	4.56057600	-1.62417900
H	-0.15326400	4.76488500	-0.79678900
Au	-2.97761700	-0.37695900	-0.19597700

Filename: AuCO2MeSO3PPh3_6
Sum of electronic and zero-point Energies = -55066.1144

Figure S58: Cartesian coordinates and energies (eV) for $[(MeCO_2)M(PPh_2C_6H_4SO_3)]^-$ in the gas phase bound through O.