

## Supplementary Materials for:

# Adsorption of Air Pollutants onto Silver and Gold Atomic Clusters: DFT and PNO-LCCSD-F12 Calculations

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**Table S1**

The XYZ coordinates of optimized structures of isolated Ag<sub>n</sub> (n = 1-22) clusters, isolated gases including CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, and SO<sub>2</sub> as well as the gas/cluster complexes at M06-2X/SDD level of theory

Ag <sub>1</sub>	X	Y	Z
47	0.00000000	0.00000000	0.00000000
Ag <sub>10</sub>			
47	0.51305200	1.59247100	1.47400800
47	0.51305200	1.59247100	-1.47400800
47	0.51305200	-1.52122800	1.45236800
47	2.62381300	0.16622200	0.00000000
47	0.51305200	-1.52122800	-1.45236800
47	1.47692900	-3.79479400	0.00000000
47	-1.52047700	-0.09008400	2.88064800
47	-1.76157400	0.32617400	0.00000000
47	-1.35042200	3.34008000	0.00000000
47	-1.52047700	-0.09008400	-2.88064800
Ag <sub>11</sub>			
47	0.00000000	0.00000000	2.69827300
47	1.53403900	1.49052300	0.65504100
47	0.00000000	4.00654800	0.94524000
47	-1.53403900	1.49052300	0.65504100
47	-1.53403900	-1.49052300	0.65504100
47	-1.47641900	0.00000000	-1.93046200
47	0.00000000	2.65895600	-1.67399500
47	1.47641900	0.00000000	-1.93046200
47	1.53403900	-1.49052300	0.65504100
47	0.00000000	-2.65895600	-1.67399500
47	0.00000000	-4.00654800	0.94524000
Ag <sub>12</sub>			
47	1.38269000	0.58475600	0.00000000
47	1.03950100	-2.36585900	0.00000000
47	0.22686800	-0.88057700	2.38954600
47	-1.23063600	1.64214300	1.45427700
47	-1.23063600	1.64214300	-1.45427700
47	-1.68996800	-0.89775700	0.00000000
47	-1.23063600	-3.39138300	-1.56177000
47	0.22686800	-0.88057700	-2.38954600
47	-1.23063600	-3.39138300	1.56177000
47	1.46447500	2.18788000	-2.49306000
47	0.80763500	3.56273300	0.00000000
47	1.46447500	2.18788000	2.49306000
Ag <sub>13</sub>			
47	0.00000000	1.68878000	0.25477800
47	1.90676100	2.41496400	2.37884500
47	0.61602100	2.43293100	-2.59343900
47	2.42112600	-0.14488000	0.95074800
47	2.77288700	2.42099300	-0.54695700
47	0.00000000	0.00000000	2.78533200
47	0.00000000	-1.68878000	0.25477800
47	-1.51612000	0.24770800	-1.83664100
47	1.51612000	-0.24770800	-1.83664100
47	-2.77288700	-2.42099300	-0.54695700
47	-2.42112600	0.14488000	0.95074800

47	-0.61602100	-2.43293100	-2.59343900
47	-1.90676100	-2.41496400	2.37884500

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 $A_{g_{14}}$   
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47	-0.73281600	1.44119500	-1.05698200
47	2.13500600	1.35521000	-0.66581100
47	1.44290400	0.19487500	-3.36702000
47	0.40345700	1.42942700	1.65789700
47	-0.40345700	-1.42942700	1.65789700
47	1.44290400	-0.36954500	3.82950500
47	-1.44290400	0.36954500	3.82950500
47	3.66060200	-0.99864300	-1.63085900
47	0.73281600	-1.44119500	-1.05698200
47	-1.44290400	-0.19487500	-3.36702000
47	2.67234900	-0.87901100	1.23326900
47	-2.13500600	-1.35521000	-0.66581100
47	-2.67234900	0.87901100	1.23326900
47	-3.66060200	0.99864300	-1.63085900

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 $A_{g_{15}}$   
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47	0.00000000	4.00940900	-0.10763400
47	1.53590300	-1.47036200	-0.36141100
47	1.53590300	1.47036200	-0.36141100
47	2.00609800	0.00000000	2.14197200
47	0.00000000	2.23573400	2.26386800
47	1.49080300	0.00000000	-2.96371000
47	-1.53590300	1.47036200	-0.36141100
47	-1.53590300	-1.47036200	-0.36141100
47	-2.00609800	0.00000000	2.14197200
47	-1.49080300	0.00000000	-2.96371000
47	0.00000000	2.62729400	-2.76942500
47	0.00000000	-2.62729400	-2.76942500
47	0.00000000	-2.23573400	2.26386800
47	0.00000000	0.00000000	4.31550400
47	0.00000000	-4.00940900	-0.10763400

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 $A_{g_{16}}$   
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47	3.64194200	0.67807000	0.00000000
47	-1.45803600	-1.34922300	2.28574700
47	1.24490500	-0.35455600	1.63251800
47	-0.94377800	1.54777700	1.62807300
47	1.81228100	2.56477100	1.54490600
47	0.44538700	-3.33815300	1.46958700
47	1.24490500	-0.35455600	-1.63251800
47	-1.45803600	-1.34922300	-2.28574700
47	-0.94377800	1.54777700	-1.62807300
47	0.44538700	-3.33815300	-1.46958700
47	2.89880800	-2.25197000	0.00000000
47	-2.21963400	-3.10697700	0.00000000
47	-3.11754500	2.77254600	0.00000000
47	-0.32525900	3.97701700	0.00000000
47	-3.07982800	-0.20991800	0.00000000
47	1.81228100	2.56477100	-1.54490600

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 $A_{g_{17}}$   
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47	-1.50020200	2.59708800	2.05610500
47	0.00000000	-3.54597700	-0.38136500
47	-2.46649600	0.00000000	-3.06153700
47	-2.90161700	0.00000000	1.83991500
47	0.00000000	1.58431600	-2.57511900
47	1.50020200	-2.59708800	2.05610500

47	0.0000000	0.0000000	2.56445500
47	0.0000000	3.54597700	-0.38136500
47	2.90161700	0.0000000	1.83991500
47	1.50020200	2.59708800	2.05610500
47	2.46649600	0.0000000	-3.06153700
47	-1.50020200	-2.59708800	2.05610500
47	0.0000000	-1.58431600	-2.57511900
47	2.26879900	1.61264900	-0.60816600
47	2.26879900	-1.61264900	-0.60816600
47	-2.26879900	1.61264900	-0.60816600
47	-2.26879900	-1.61264900	-0.60816600

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 $A_{g_{18}}$   
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47	-0.01226300	-3.57910100	0.00000000
47	-2.49800700	3.25888400	0.00000000
47	0.01273700	0.25781700	3.21022400
47	3.48485800	-1.41237200	0.00000000
47	-1.47317700	-2.14656500	2.23835800
47	-2.46537700	0.75582800	1.63376300
47	2.42629000	0.82746500	1.59576300
47	-0.05058600	2.64731600	-1.54105700
47	2.42629000	0.82746500	-1.59576300
47	-1.47317700	-2.14656500	-2.23835800
47	1.55639200	-2.08898200	-2.13575800
47	-3.29472400	-1.56693200	0.00000000
47	0.01273700	0.25781700	-3.21022400
47	2.38118400	3.34550200	0.00000000
47	1.55639200	-2.08898200	2.13575800
47	-2.46537700	0.75582800	-1.63376300
47	-0.05058600	2.64731600	1.54105700
47	-0.07360700	-0.55174200	0.00000000

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 $A_{g_{19}}$   
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47	0.65027600	-2.76104400	2.58635200
47	0.54734500	2.34155900	-2.54517900
47	-0.20382000	4.01291500	0.00000000
47	-2.41918900	2.30404200	-1.57711400
47	2.57671900	-2.56625600	0.00000000
47	-2.41918900	2.30404200	1.57711400
47	-0.24273800	1.11136900	0.00000000
47	-2.47590600	-2.75007600	1.65205800
47	-1.09695500	-0.25050100	2.58324300
47	1.93725900	-0.20729500	-1.78480200
47	0.54734500	2.34155900	2.54517900
47	-2.47590600	-2.75007600	-1.65205800
47	0.65027600	-2.76104400	-2.58635200
47	-1.09695500	-0.25050100	-2.58324300
47	2.43951000	2.28016100	0.00000000
47	-2.91947600	-0.27491900	0.00000000
47	4.31327100	-0.07259700	0.00000000
47	1.93725900	-0.20729500	1.78480200
47	-0.24912400	-1.84404300	0.00000000

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 $A_{g_{20}}$   
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47	0.46400700	-2.51855000	1.41938400
47	0.00000000	0.00000000	-0.54544700
47	0.01355400	1.73933200	-3.25328400
47	0.00000000	2.97669200	-0.49211200
47	2.50215900	1.42455600	-1.51556100
47	4.53486900	0.50918500	0.53695500
47	-2.48478100	1.45465500	-1.51556100
47	-2.70840200	3.67271900	0.53695500

47	1.49952900	-0.88140400	-3.25328400
47	1.94912500	1.66111700	1.41938400
47	2.57789100	-1.48834600	-0.49211200
47	2.79536500	-1.02924300	2.48413600
47	-1.82646700	-4.18190400	0.53695500
47	-2.28903300	-1.90623600	2.48413600
47	-2.57789100	-1.48834600	-0.49211200
47	-2.41313200	0.85743300	1.41938400
47	-1.51308300	-0.85792800	-3.25328400
47	-0.50633200	2.93547900	2.48413600
47	-0.01737800	-2.87921100	-1.51556100
47	0.00000000	0.00000000	3.00689300

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 $A_{g_{21}}$   
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47	0.00000000	4.52915700	-2.26504500
47	2.56866100	1.53504100	1.14118100
47	2.45232700	2.93904900	-1.47038700
47	2.45232700	-2.93904900	-1.47038700
47	0.00000000	1.48009700	-2.52568700
47	-2.45232700	-2.93904900	-1.47038700
47	0.00000000	-1.48009700	-2.52568700
47	-2.58864500	0.00000000	-1.51225200
47	0.00000000	0.00000000	0.16792700
47	2.58864500	0.00000000	-1.51225200
47	2.56866100	-1.53504100	1.14118100
47	0.00000000	3.05647700	0.31155300
47	-2.43240900	0.00000000	3.71400900
47	0.00000000	-1.52797400	2.85187100
47	-2.56866100	1.53504100	1.14118100
47	0.00000000	1.52797400	2.85187100
47	-2.56866100	-1.53504100	1.14118100
47	-2.45232700	2.93904900	-1.47038700
47	2.43240900	0.00000000	3.71400900
47	0.00000000	-4.52915700	-2.26504500
47	0.00000000	-3.05647700	0.31155300

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 $A_{g_{22}}$   
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47	1.53936000	-2.72727100	-0.77766500
47	-0.72245500	-0.95367800	0.15690400
47	4.55298700	1.31132600	-0.30970900
47	1.34240500	-1.67470100	2.27793800
47	4.09537900	-1.45050600	0.50802300
47	-0.71957300	-3.68020700	1.15052800
47	3.01762400	0.87106700	2.53941300
47	-1.55597300	-1.30645700	2.98531800
47	-3.47721700	-1.89798900	0.38742800
47	-2.79407600	0.93012800	1.16274100
47	-2.64298900	-0.05816800	-1.97717500
47	-3.35215400	2.75272500	-1.14494900
47	-1.40185300	-2.90939100	-1.92427600
47	-5.25306200	0.32875000	-0.48176300
47	-0.53451800	1.84962500	-1.00697100
47	0.27655400	-0.53320800	-2.77807900
47	1.85593300	0.24011200	-0.11974800
47	3.24380100	-0.86356700	-2.51459200
47	0.04283100	1.16396300	2.38331800
47	2.16872200	1.98651500	-2.40863200
47	-1.37325500	3.56524300	1.23125800
47	1.69152900	3.05568900	0.66069000

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 $A_{g_2}$   
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47	0.00000000	0.00000000	1.33867400
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47 0.0000000 0.0000000 -1.33867400

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Ag<sub>3</sub>  
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47 1.68687800 -0.60509400 0.00000000  
47 -1.68687800 -0.79457000 0.00000000  
47 0.00000000 1.39966500 0.00000000

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Ag<sub>4</sub>  
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47 0.00000000 0.00000000 2.54990000  
47 0.00000000 1.37154700 0.00000000  
47 0.00000000 -1.37154700 0.00000000  
47 0.00000000 0.00000000 -2.54990000

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Ag<sub>5</sub>  
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47 0.00000000 0.00000000 1.05810500  
47 0.00000000 1.45469500 -1.51144400  
47 0.00000000 -1.45469500 -1.51144400  
47 0.00000000 2.83948500 0.98239100  
47 0.00000000 -2.83948500 0.98239100

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Ag<sub>6</sub>  
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47 0.00000000 1.72635300 0.00000000  
47 2.83144500 1.63473600 0.00000000  
47 1.49506600 -0.86317700 0.00000000  
47 0.00000000 -3.26947100 0.00000000  
47 -1.49506600 -0.86317700 0.00000000  
47 -2.83144500 1.63473600 0.00000000

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Ag<sub>7</sub>  
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47 0.00000000 2.51118600 0.00000000  
47 2.38828000 0.77599900 0.00000000  
47 1.47603800 -2.03159200 0.00000000  
47 0.00000000 0.00000000 1.61426500  
47 0.00000000 0.00000000 -1.61426500  
47 -1.47603800 -2.03159200 0.00000000  
47 -2.38828000 0.77599900 0.00000000

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Ag<sub>8</sub>  
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47 0.00000000 1.97682600 0.61488700  
47 -1.97682600 0.00000000 -0.61488700  
47 0.00000000 1.54406000 -2.22525300  
47 0.00000000 -1.54406000 -2.22525300  
47 1.97682600 0.00000000 -0.61488700  
47 0.00000000 -1.97682600 0.61488700  
47 -1.54406000 0.00000000 2.22525300  
47 1.54406000 0.00000000 2.22525300

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Ag<sub>9</sub>  
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47 -1.30726900 -2.60419500 0.00000000  
47 0.25875500 -0.99278900 1.97384400  
47 -1.74652200 0.22717500 0.00000000  
47 1.73460600 -2.73915400 0.00000000  
47 0.25875500 -0.99278900 -1.97384400  
47 0.25875500 1.85663300 -1.55612900  
47 2.20067500 0.20662000 0.00000000  
47 0.25875500 1.85663300 1.55612900  
47 -1.91651100 3.18186500 0.00000000

CH<sub>4</sub>\_Ag<sub>10</sub>

47	0.99009900	1.52323700	1.28421000
47	1.47354200	-1.35501600	0.78412600
47	-1.88532900	1.26263300	0.11254700
47	-0.82275700	-0.48706100	2.41911700
47	-1.41846400	-1.56070500	-0.38210800
47	-4.09004700	-0.53434700	-0.21143200
47	-0.07330300	3.20624500	-0.95684200
47	0.85599900	0.48515700	-1.50001600
47	3.49748700	0.64403400	0.00984800
47	0.83455800	-2.39583400	-1.95198600
6	2.99760400	-3.70309600	1.84360000
1	3.58148900	-4.53289200	2.25119700
1	2.94612400	-2.90617700	2.59346100
1	3.49192100	-3.33369500	0.93852900
1	1.99090000	-4.06076500	1.60440200

CH<sub>4</sub>\_Ag<sub>11</sub>

47	0.00771200	-2.63650100	-0.43313100
47	1.64903500	-0.45069300	-1.59928300
47	4.02993500	-1.03781400	0.05155800
47	1.42158700	-0.86348700	1.44891900
47	-1.56319100	-0.79321400	1.27249000
47	-0.00525500	1.73870100	1.64271400
47	2.74858000	1.60113900	0.34170600
47	0.21856800	2.14107300	-1.28069200
47	-1.32130100	-0.36165000	-1.76163100
47	-2.55605500	1.76257700	-0.00376300
47	-3.95480400	-0.78133500	-0.50122400
6	-3.17054500	-1.49784200	3.86410900
1	-3.55309100	-0.54810500	3.47698900
1	-3.74391000	-1.78301300	4.75058100
1	-3.27964200	-2.27690000	3.10188700
1	-2.11624300	-1.38843100	4.13582500

CH<sub>4</sub>\_Ag<sub>12</sub>

47	0.94084400	-0.04842400	-1.16065500
47	-1.97697300	-0.09504800	-1.64080600
47	-0.73921300	-2.49702600	-0.48626500
47	1.26966600	-1.55022800	1.62111400
47	1.23201300	1.35961300	1.65478400
47	-1.31117300	-0.12476200	1.36715000
47	-3.62425400	1.38968200	0.27747800
47	-0.81476300	2.30371800	-0.42912000
47	-3.54963700	-1.73814800	0.24424800
47	2.50111200	2.44852500	-0.76856600
47	3.65214300	-0.05160500	0.20598000
47	2.53700800	-2.53306700	-0.84532800
6	-0.54945100	5.34038100	-0.18797000
1	-0.20159500	4.99038600	-1.16648700
1	-1.59681700	5.05990100	-0.03955800
1	0.06954000	4.90590600	0.60420400
1	-0.46279900	6.42974300	-0.15108100

CH<sub>4</sub>\_Ag<sub>13</sub>

47	1.17279100	-0.34474300	1.08570400
47	2.68787700	-2.77861300	0.42427000
47	2.48729300	2.34157100	0.80913100
47	1.28354300	-1.42975600	-1.82755500
47	3.62616100	-0.03676000	-0.56212800
47	-0.41006000	-2.81524100	0.28963700

47	-1.35422000	-0.29477400	-1.14276200
47	-0.63273500	2.00040900	1.01089500
47	0.98698400	1.48262700	-1.54251400
47	-3.60033200	0.99686300	0.32008800
47	-1.64719000	-0.58383900	1.94612300
47	-1.93220000	2.63703900	-1.52741500
47	-3.40112400	-2.05005000	0.05420700
6	3.44517300	4.11231800	3.11117200
1	2.67704000	3.44857300	3.51997200
1	4.26998800	3.51964700	2.70145700
1	3.01229100	4.74517300	2.32920000
1	3.83062700	4.75025800	3.91135400

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CH<sub>4</sub>\_Ag<sub>14</sub>  
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47	-1.22354200	-0.83234100	1.18922000
47	-0.44626500	1.92665700	1.67411900
47	-3.12272000	1.84348100	0.28056600
47	1.61638000	-0.08829200	1.46346000
47	1.75005200	-0.30435600	-1.50519100
47	4.03996300	0.97056200	0.04630100
47	3.61815900	-1.97588300	0.16365200
47	-1.04319100	3.99964400	-0.36600600
47	-0.79392300	1.16510100	-1.34587900
47	-3.45573300	-0.88005400	-0.69826000
47	1.66555500	2.62787000	-0.31344400
47	-0.77855600	-1.68046300	-1.83651200
47	0.85919500	-2.90276400	0.32237100
47	-2.10361700	-3.50889700	0.08001600
6	-2.73422100	-1.69270700	3.97430800
1	-3.24706000	-2.05121400	4.87144900
1	-2.24014700	-0.74115800	4.18912800
1	-1.98543600	-2.42956200	3.66621100
1	-3.46463100	-1.55419000	3.16995100

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CH<sub>4</sub>\_Ag<sub>15</sub>  
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47	1.61327900	-3.60860800	0.00154500
47	-0.35309300	1.51244500	-1.53578700
47	0.83041200	-1.18087800	-1.53151300
47	-2.05395500	-0.83311800	-1.99756800
47	-1.27689300	-2.93407000	0.00032100
47	2.62301400	1.20544900	-1.48724600
47	0.83000800	-1.18004500	1.53300900
47	-0.35345900	1.51321800	1.53528800
47	-2.05462000	-0.83199800	1.99662700
47	2.62293700	1.20631800	1.48944500
47	3.50071400	-1.28162700	0.00196400
47	1.39018800	3.53902500	0.00016600
47	-3.08051800	1.17360000	-0.00123100
47	-4.05735200	-1.68934300	-0.00055200
47	-1.60137500	3.73831400	-0.00098000
6	6.67654800	-1.63862300	-0.01637900
1	6.24795800	-2.08760500	0.88527300
1	6.23570500	-2.10141500	-0.90506000
1	6.47294000	-0.56368200	-0.02332900
1	7.75763800	-1.80364600	-0.02252300

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CH<sub>4</sub>\_Ag<sub>16</sub>  
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47	0.12281200	3.64808400	0.08281400
47	0.86669600	-1.81977300	2.28155100
47	0.54854900	1.04780400	1.64630300
47	-1.81846200	-0.64302700	1.60257700
47	-2.16394900	2.27225900	1.56594700



47	3.26087900	-0.42507300	1.51672400
47	0.59514400	1.10214500	-1.57987800
47	0.93564300	-1.74548800	-2.29265300
47	-1.77115900	-0.58440200	-1.65801200
47	3.30395100	-0.37930200	-1.41642000
47	2.80971200	2.24815800	0.09019600
47	2.42889000	-2.94047100	-0.00192100
47	-3.49977600	-2.44035900	-0.08932800
47	-4.01154600	0.55177800	-0.03987400
47	-0.58885900	-3.08937200	-0.05140800
47	-2.11638900	2.32722700	-1.52428300
6	5.15823400	4.08629600	-0.62159800
1	5.98084000	4.77269000	-0.84046200
1	4.63832300	4.43258300	0.27822500
1	4.46662500	4.07509700	-1.47005900
1	5.56430600	3.08306300	-0.45772800

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CH<sub>4</sub>\_Ag<sub>17</sub>  
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47	-2.46466900	-2.12236100	-1.50501100
47	3.62701800	0.46408000	0.00713900
47	0.01614300	3.06299000	-2.46070000
47	0.13611600	-1.84462100	-2.90491200
47	-1.57085900	2.53705100	-0.00128500
47	2.72690600	-1.99555300	1.50411200
47	0.14359000	-2.53842200	-0.00123400
47	-3.48969000	0.30035600	-0.00706700
47	0.12284200	-1.84854600	2.90290900
47	-2.47199400	-2.12331700	1.49258400
47	0.00654100	3.05978200	2.46432100
47	2.73309400	-1.99317000	-1.49573400
47	1.60947400	2.61965300	0.00430800
47	-1.53854100	0.55919000	2.23767000
47	1.66658400	0.64035900	2.25772900
47	-1.52801800	0.56155100	-2.24181400
47	1.67732900	0.64394900	-2.25260700
6	-6.58716500	0.07995400	-0.00189800
1	-7.68072500	0.07280500	0.00552200
1	-6.21985700	-0.06198300	1.01952800
1	-6.22513400	-0.73200100	-0.64016000
1	-6.23885500	1.04181200	-0.39263300

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CH<sub>4</sub>\_Ag<sub>18</sub>  
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47	-3.60119900	-0.05337900	0.53669600
47	3.22401500	2.40319300	-0.55163200
47	0.69131300	-0.00541100	3.09139300
47	-1.59973800	-3.28294600	0.19930100
47	-1.80385200	1.53503500	2.40737600
47	0.99845400	2.40690200	1.42410300
47	0.95443700	-2.47116700	1.44456100
47	2.29963900	-0.02499200	-1.97148200
47	0.42220500	-2.44690000	-1.79910600
47	-2.46753200	1.56252500	-1.76372600
47	-2.53733500	-1.45950500	-1.91915200
47	-1.45440900	3.50755900	0.22624300
47	-0.32077300	0.04856500	-3.24728600
47	3.15288300	-2.48879200	-0.57820200
47	-1.83192700	-1.49859600	2.53230400
47	0.48243100	2.44022900	-1.71999000
47	2.79642500	-0.05109100	1.06654100
47	-0.60742600	-0.10357900	0.06585200
6	5.65108500	-0.08287800	2.61418200
1	6.60796300	-0.09169600	3.14392300
1	5.07617200	-0.97342000	2.88619300

1	5.08900000	0.81411300	2.89163400
1	5.83271500	-0.08124200	1.53486800

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CH<sub>4</sub>\_Ag<sub>19</sub>  
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47	2.29511000	0.94975700	2.91838000
47	-1.86525100	0.26559500	-2.95557600
47	-3.87735100	-0.52510000	-0.67804000
47	-1.78203800	-2.65501800	-1.84342500
47	2.40168900	2.75630100	0.23621800
47	-2.30107900	-2.53379500	1.27093900
47	-1.02142200	-0.33295800	-0.20212400
47	2.65060400	-2.19775300	2.15849100
47	-0.05366100	-0.97405300	2.60410900
47	0.42614900	1.86574400	-1.87159400
47	-2.71154300	0.46353200	2.05350200
47	3.20635500	-2.32209400	-1.12241200
47	3.15769900	0.72444000	-2.20169700
47	0.79602300	-1.17617400	-2.48844000
47	-2.36154700	2.24727100	-0.53290700
47	0.53273000	-2.89483100	0.14558000
47	-0.17442000	4.29285200	-0.26345500
47	-0.16983000	2.00631500	1.64442900
47	1.89757800	-0.11419100	0.26174800
6	-4.91253700	0.72405300	4.06880400
1	-5.70304800	0.86523500	4.81129700
1	-4.33703800	-0.17037400	4.33148000
1	-5.37350800	0.59904400	3.08263200
1	-4.26347700	1.60721700	4.07663300

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CH<sub>4</sub>\_Ag<sub>1</sub>  
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6	-2.85006300	0.00001900	-0.00003000
1	-3.94310700	-0.00419500	0.00792500
1	-2.47660500	-0.18412400	1.01158800
1	-2.48637100	-0.78433400	-0.67032100
1	-2.49069400	0.97256200	-0.34904200
47	0.60632300	0.00000000	0.00000100

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CH<sub>4</sub>\_Ag<sub>20</sub>  
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47	-2.49442000	0.98448400	-1.26201400
47	-0.01028300	-0.00181100	0.55265300
47	1.84600300	-0.35771400	3.13405100
47	2.88913500	-0.65155500	0.30467400
47	1.97729600	2.13909600	1.38053400
47	1.39481200	4.31000600	-0.65959500
47	0.91328700	-2.73856900	1.45941600
47	2.87711200	-3.45301900	-0.73244000
47	-0.38192900	1.66765800	3.26989500
47	1.86082800	1.52413300	-1.54849800
47	-0.90563500	2.83916800	0.52932500
47	-0.62663700	2.94556300	-2.47289600
47	-4.58225500	-0.85244000	-0.24384200
47	-2.58899400	-1.83017300	-2.32389000
47	-2.05100400	-2.17393900	0.62070700
47	0.14468600	-2.53453800	-1.42869700
47	-1.01961900	-1.27989300	3.31984000
47	2.51835400	-1.14093800	-2.65680000
47	-2.77081000	0.62367000	1.69081700
47	-0.26745700	-0.01372300	-3.01916200
6	6.00337700	-0.02554600	0.40374700
1	7.08446200	0.12577700	0.46981300
1	5.55820300	0.78191900	-0.18531300
1	5.80424600	-0.98715700	-0.08068400

1 5.57670400 -0.02413700 1.41202900

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CH<sub>4</sub>\_Ag<sub>21</sub>  
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47 -4.50082400 -2.14759000 -0.75796700  
47 -1.57510800 1.96673700 -2.05582300  
47 -2.94709500 -0.55477600 -2.81244400  
47 2.92647500 -0.46255100 -2.84293500  
47 -1.45237400 -2.35473900 -0.85624400  
47 2.97940100 -2.08678800 1.77795300  
47 1.50561500 -2.30810000 -0.87825400  
47 0.03679100 -2.25157000 1.93422600  
47 -0.00217300 0.19147300 0.03960400  
47 -0.01178300 -0.50888300 -2.96935500  
47 1.48728600 2.01383000 -2.06619300  
47 -3.06374700 0.30812500 0.09066700  
47 -0.02500300 2.74270000 3.50689400  
47 1.48190600 2.76827700 0.91263800  
47 -1.52393100 0.24927400 2.78329300  
47 -1.55787200 2.71753100 0.92626000  
47 1.53585900 0.29456000 2.77363700  
47 -2.90552600 -2.18493900 1.81269100  
47 -0.07906300 4.37613000 -1.09856600  
47 4.54512600 -2.01532000 -0.80548400  
47 3.05281800 0.40694500 0.05820100  
6 0.43860000 -5.45353800 2.47781100  
1 -0.59130600 -5.08378300 2.52548300  
1 0.45251500 -6.51762500 2.72970400  
1 0.82947200 -5.31089300 1.46554900  
1 1.05920300 -4.90176600 3.19098600

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CH<sub>4</sub>\_Ag<sub>22</sub>  
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47 -1.48701800 -2.63038400 1.19707300  
47 0.76809400 -0.99935200 -0.00825100  
47 -4.55807700 1.19717200 -0.01445100  
47 -1.25807100 -2.13259000 -1.97719100  
47 -4.04285200 -1.66356900 -0.33223800  
47 0.82032900 -3.86448000 -0.51053800  
47 -2.97634200 0.28530000 -2.72100500  
47 1.64089500 -1.85054900 -2.70882400  
47 3.55020600 -1.88831600 -0.01898800  
47 2.81524200 0.72584000 -1.31253900  
47 2.62381300 0.31624400 1.96255100  
47 3.29570800 2.94440000 0.65316300  
47 1.44547600 -2.53707000 2.39226100  
47 5.25258600 0.51275300 0.45781900  
47 0.50057500 1.96327000 0.62443400  
47 -0.30192400 -0.08430100 2.78135500  
47 -1.84524400 0.16470100 0.02369100  
47 -3.25606300 -0.50634400 2.55259500  
47 -0.00663100 0.66399600 -2.59136800  
47 -2.23815100 2.29592500 1.93452400  
47 1.33600200 3.26688200 -1.87515200  
47 -1.73093800 2.79385300 -1.25281300  
6 -1.63371500 4.82313000 3.49451700  
1 -1.55480400 5.72922900 4.10177700  
1 -1.71176900 5.10560600 2.43971400  
1 -0.74181200 4.20780800 3.64664300  
1 -2.52716100 4.26966400 3.80771600

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CH<sub>4</sub>\_Ag<sub>2</sub>  
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6 -3.87321200 0.00803200 -0.00155600  
1 -3.51905300 -0.84826000 -0.58555900

1	-3.52384800	0.94375600	-0.45083500
1	-4.96652700	0.00492300	-0.00373600
1	-3.52420800	-0.06866500	1.03376900
47	-0.92350300	-0.00357900	0.00070300
47	1.74845800	0.00187800	-0.00036900

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CH<sub>4</sub>\_Ag<sub>3</sub>  
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6	-3.53069700	1.55988100	-0.00090400
1	-3.66381400	0.96887400	0.91118300
1	-2.51722000	1.97445800	-0.03223700
1	-3.70510700	0.93332200	-0.88171400
1	-4.25138400	2.38205300	-0.00056500
47	0.97538600	1.60081200	0.00013200
47	-1.46488700	-0.74319800	0.00031700
47	1.24102600	-1.18991200	-0.00026300

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CH<sub>4</sub>\_Ag<sub>4</sub>  
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47	-2.84797300	-0.01055600	0.00779200
47	-0.29658200	1.36990800	-0.00231800
47	-0.28418600	-1.36586500	-0.00274600
47	2.26311100	0.01481000	-0.01109400
6	5.47785800	-0.03901700	0.03938800
1	6.57129500	-0.05266300	0.04839200
1	5.13084900	0.90667300	-0.38822100
1	5.10988900	-0.87238300	-0.56689800
1	5.10544900	-0.13748700	1.06358900

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CH<sub>4</sub>\_Ag<sub>5</sub>  
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47	-0.37925600	-1.16001000	-0.00279100
47	-1.25774700	1.65517300	0.00673600
47	1.58540900	1.02415000	0.00539400
47	-3.14281300	-0.50015800	-0.00525200
47	2.40563800	-1.70934300	0.00188300
6	3.70549400	3.24231000	-0.02828600
1	4.50463600	3.98843900	-0.04264600
1	2.88972300	3.57735700	-0.67642300
1	4.10475700	2.28843800	-0.38958600
1	3.34003900	3.13077800	0.99775900

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CH<sub>4</sub>\_Ag<sub>6</sub>  
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47	0.64824200	-1.48200300	-0.00371300
47	-1.85087100	-2.82755000	0.00228300
47	-1.95656800	0.00098500	0.00258900
47	-1.84769000	2.82936000	0.00218100
47	0.65007500	1.48122500	-0.00353500
47	3.06372400	-0.00209600	-0.00559100
6	6.07445200	0.00041300	0.02720400
1	7.16777600	-0.00062500	0.03614300
1	5.72748000	0.66419100	-0.77152100
1	5.72071200	-1.02014100	-0.15270500
1	5.71247100	0.35782000	0.99680900

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CH<sub>4</sub>\_Ag<sub>7</sub>  
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47	-1.16286900	2.22516200	-0.10170500
47	1.75221700	1.79361700	-0.14161300
47	2.24175800	-1.11308200	-0.17696300
47	0.01537900	-0.01587600	1.47600700
47	-0.02091900	0.02180900	-1.77124300
47	-0.37271800	-2.47590300	-0.16432100
47	-2.47609900	-0.41214300	-0.11969000

6	0.10921700	-0.11084900	4.69700900
1	1.00060400	0.40437500	4.32627200
1	-0.78766400	0.42664600	4.37354000
1	0.08675700	-1.13273300	4.30620800
1	0.13773800	-0.14165100	5.78975200

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CH<sub>4</sub>\_Ag<sub>8</sub>  
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47	0.46166300	0.14501700	-1.96859200
47	-1.15022700	1.85869100	-0.00051500
47	-2.32883500	-0.39969700	-1.53234500
47	-2.32898800	-0.39864500	1.53224400
47	-0.33580900	-2.02361200	0.00004500
47	0.46141600	0.14490500	1.96905000
47	1.72092800	1.99089900	-0.00013200
47	2.35954000	-1.03351000	0.00046500
6	5.35646300	-1.33449800	-0.00104000
1	6.43936800	-1.48567400	0.00061600
1	5.07747300	-0.77211400	-0.89803100
1	4.86423000	-2.31314100	-0.00196400
1	5.07480300	-0.77238600	0.89531700

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CH<sub>4</sub>\_Ag<sub>9</sub>  
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47	1.83149400	2.20057700	-0.29520200
47	1.10618700	-0.16548900	-1.94873100
47	-0.92800400	1.38791000	-0.22886300
47	3.28621200	-0.45705100	0.11065400
47	1.02526300	0.38137900	1.92048100
47	-1.52023600	-0.91871300	1.64542000
47	0.85045300	-2.16023900	0.29700100
47	-1.45732300	-1.34569100	-1.42850200
47	-3.64583600	0.18059000	-0.12355400
6	-2.57645500	4.21475200	0.24119700
1	-3.13623300	5.14868200	0.34330800
1	-2.83291800	3.54320200	1.06625200
1	-2.83479300	3.74021800	-0.71124300
1	-1.50315400	4.42555700	0.26541100

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CH<sub>4</sub>  
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6	0.00000000	0.00000000	0.00000000
1	0.63093600	0.63093600	0.63093600
1	-0.63093600	-0.63093600	0.63093600
1	-0.63093600	0.63093600	-0.63093600
1	0.63093600	-0.63093600	-0.63093600

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CO<sub>2</sub>\_Ag<sub>10</sub>  
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47	-0.76939500	1.58597300	1.24457600
47	2.14093100	1.07692800	0.21489800
47	-1.48494200	-1.22118900	0.61043800
47	0.77886900	-0.61688400	2.40088700
47	1.41265100	-1.67745900	-0.38175500
47	-0.80614500	-2.22015800	-2.12181100
47	-3.25122800	1.05206900	-0.25230300
47	-0.54141000	0.62463300	-1.56477800
47	0.59874600	3.22537400	-0.87344800
47	4.14849800	-0.95759400	0.07596600
6	-4.75823100	-1.85734300	1.38162500
8	-5.82590600	-1.35670000	1.43196400
8	-3.68655200	-2.37148800	1.33487900

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CO<sub>2</sub>\_Ag<sub>11</sub>  
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47	0.16672600	-2.48110600	-1.05418000
47	-1.24310400	-1.42388100	1.36993200
47	-3.65688800	-1.62213000	-0.33452400
47	-1.35355500	0.00257900	-1.48377300
47	1.64361800	-0.06702400	-1.56822700
47	0.27407100	2.51959400	-0.91296700
47	-3.11318700	0.89293700	0.89998400
47	0.01806500	1.16406000	1.73397100
47	1.68975800	-1.28606800	1.28898700
47	2.70768100	1.64529100	0.49742300
47	4.22514700	-0.74485100	-0.05533600
6	-2.95813300	2.76705800	-0.57822100
8	-2.06276600	2.43430700	-1.44164100
8	-3.69883400	3.71892200	-0.36477500

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CO<sub>2</sub>\_Ag<sub>12</sub>  
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47	-0.92030000	0.14365500	0.98059300
47	2.06271700	0.20971800	1.43099300
47	0.73277800	-2.34854700	0.80885400
47	-1.35848400	-1.84472800	-1.40549400
47	-1.34184500	0.99328900	-2.02327600
47	1.23808600	-0.40907800	-1.49395400
47	3.57310500	1.32979900	-0.82459900
47	0.79678300	2.32138000	-0.24943600
47	3.54904900	-1.73678500	-0.12116600
47	-2.40610300	2.55808400	0.25583000
47	-3.67630000	-0.04751700	-0.25664600
47	-2.53453700	-2.30276300	1.25757300
6	0.60658500	2.42362700	3.50804500
8	1.55323700	1.70544100	3.56261500
8	-0.33350900	3.13611200	3.44563200

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CO<sub>2</sub>\_Ag<sub>13</sub>  
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47	1.28474100	-0.04704900	-1.21437300
47	3.57918800	1.71645900	-0.73764800
47	1.68203100	-3.01722900	-1.00440300
47	2.04415400	0.88420300	1.68908600
47	3.64836800	-1.17192900	0.23525100
47	0.71368100	2.78642100	-0.28626900
47	-0.87713900	0.71504700	1.24798000
47	-1.14575500	-1.68084400	-0.93337700
47	0.74820700	-1.74328700	1.47129000
47	-3.59205500	0.34496200	0.08198600
47	-1.37702400	1.12848100	-1.76950600
47	-2.39583900	-1.80684700	1.74954400
47	-2.29593700	3.10536900	0.27816100
6	-4.31158100	-2.59485100	-1.72556900
8	-5.38745200	-2.16274600	-1.49641500
8	-3.22651200	-3.02193600	-1.95476600

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CO<sub>2</sub>\_Ag<sub>14</sub>  
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47	-1.11114400	1.12388500	-1.36612700
47	-0.77741900	-1.69475600	-1.92989700
47	-3.43390300	-1.32344200	-0.54529800
47	1.58065400	-0.02385900	-1.64468600
47	1.71072400	0.12128400	1.31909800
47	3.80531100	-1.45562400	-0.21212100
47	3.81296500	1.52664000	-0.26719800
47	-1.65637200	-3.73805700	0.04175500
47	-1.05587000	-0.97970200	1.10184700
47	-3.35079700	1.40023800	0.48943500
47	1.20258600	-2.74604000	0.05579600

47	-0.62019800	1.81096900	1.69204300
47	1.21624400	2.85155200	-0.40404700
47	-1.64136200	3.84893100	-0.21927100
6	0.67966400	-1.54280300	4.03906300
8	1.77724000	-1.09468200	3.97764300
8	-0.41533400	-1.99006900	4.08900400

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CO<sub>2</sub>\_Ag<sub>15</sub>  
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47	4.16389800	0.85390900	0.00084200
47	-1.12676800	-0.68157400	1.52142200
47	1.74008200	0.01430200	1.53620100
47	-0.27795600	2.09454100	2.01494800
47	1.86230600	2.72810000	-0.00012600
47	0.93032900	-2.85672700	1.48942300
47	1.74253400	0.01503100	-1.53907600
47	-1.12470000	-0.68184200	-1.51650600
47	-0.27845100	2.09396800	-2.01460800
47	0.93199900	-2.85660400	-1.49102600
47	3.43701300	-2.04336700	0.00030500
47	-1.67659400	-3.28748500	0.00020000
47	-2.47486100	1.67912500	0.00058400
47	-0.79357600	4.19816100	-0.00058100
47	-3.66072100	-1.04281700	0.00063300
6	-7.25467200	-0.48333600	-0.00545400
8	-8.29147800	0.07966000	-0.00778400
8	-6.21041100	-1.04913600	-0.00360100

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CO<sub>2</sub>\_Ag<sub>16</sub>  
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47	0.66180500	3.45014100	-0.79816000
47	-1.28104900	-2.04279300	-2.07176000
47	-0.31749200	0.73133200	-1.77823700
47	1.62170800	-1.40213000	-1.49829800
47	2.58744300	1.34345400	-1.93737800
47	-3.30085400	-0.03335600	-1.65959900
47	-0.41956000	1.45981900	1.42140000
47	-1.37526900	-1.15781100	2.42464100
47	1.49175500	-0.70588300	1.66837300
47	-3.35610000	0.52920900	1.21626100
47	-2.26330000	2.67946500	-0.65754400
47	-3.07852700	-2.36665500	0.29186400
47	2.81544200	-3.14709600	0.60216800
47	3.98819000	-0.40608300	0.04588900
47	-0.16823900	-3.15778800	0.50414800
47	2.51076800	1.97875800	1.09614700
6	-0.24707600	4.80240000	2.41239300
8	0.29956400	5.80767200	2.11858400
8	-0.80000200	3.79411400	2.71136900

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CO<sub>2</sub>\_Ag<sub>17</sub>  
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47	-1.33909200	-2.31768300	-2.50380300
47	2.81864500	0.82682300	1.80017700
47	0.67297200	3.14888300	-2.18370500
47	1.55821700	-1.71597300	-2.39620500
47	-1.86032600	2.35477300	-0.84795200
47	1.57748500	-1.76269600	2.72915200
47	0.18163000	-2.51439000	0.12992500
47	-3.22387500	-0.08698000	-1.76534300
47	-1.37310800	-1.93949900	2.61173600
47	-2.84702000	-2.44049900	0.09270700
47	-1.79574600	2.94111900	2.06916900
47	3.08883000	-1.66273300	0.13587200
47	0.84999300	2.74649000	0.75021500

47	-2.71924200	0.30081700	1.15324800
47	0.00217300	0.72384100	2.80440200
47	-0.45801000	0.48299200	-2.73450300
47	2.26474000	0.90580500	-1.13368800
6	5.56241400	0.01988000	-1.52126600
8	5.97866700	-0.91062600	-0.91658100
8	5.13470500	0.94806300	-2.12197400

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CO<sub>2</sub>\_Ag<sub>18</sub>  
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47	3.74152600	-0.06414700	0.00165000
47	-3.15871800	-2.45914700	-0.00421800
47	-0.08805500	0.01942800	3.20333200
47	1.58671000	3.50434700	0.00383900
47	2.29352200	-1.49510200	2.24727400
47	-0.63368400	-2.46494700	1.62120600
47	-0.66619300	2.42974800	1.57602800
47	-2.46482400	-0.03065400	-1.53951400
47	-0.66469600	2.43380600	-1.57253400
47	2.29617700	-1.48821700	-2.24811200
47	2.25599200	1.55296600	-2.10831700
47	1.70223100	-3.29404600	-0.00260100
47	-0.08480400	0.02614100	-3.20347700
47	-3.20860300	2.39096000	0.00057200
47	2.25351700	1.54830800	2.11300600
47	-0.63179900	-2.46148600	-1.62628000
47	-2.46714800	-0.03381900	1.53770300
47	0.71807200	-0.10274900	-0.00001800
6	-5.94474800	-0.02451300	0.00088400
8	-5.89816700	1.16047800	0.00218400
8	-5.97122000	-1.20900900	-0.00013200

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CO<sub>2</sub>\_Ag<sub>19</sub>  
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47	1.43214600	2.48463700	2.52131800
47	-1.60072300	-1.40609900	-2.76908900
47	-2.86446300	-2.73894100	-0.22140000
47	0.07040300	-3.54394100	-1.24209200
47	0.56410400	3.54350600	-0.39526800
47	-0.46949800	-3.16866500	1.84966800
47	-0.60521600	-0.93378900	-0.05464100
47	3.48794500	-0.04106900	2.21779700
47	0.54725300	-0.43095900	2.71688200
47	-0.58712500	1.34923700	-2.14373000
47	-2.46134900	-0.78548600	2.21515400
47	4.05691700	-0.43548100	-0.96518600
47	2.30708800	1.87327500	-2.53792800
47	1.42908700	-1.04884600	-2.32555500
47	-3.14956100	0.36862900	-0.70134400
47	2.09693000	-2.12788000	0.56029800
47	-2.41453300	3.33015300	-0.90697600
47	-1.20213100	1.78414400	1.32203800
47	1.70814700	0.91153900	0.11621900
6	-5.01057400	2.17291200	1.59138800
8	-5.27211800	1.41358500	0.71372400
8	-4.74929900	2.92594300	2.46277700

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CO<sub>2</sub>\_Ag<sub>1</sub>  
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6	-0.00194900	-2.74025600	0.00000000
8	-0.25134000	-1.58006700	0.00000000
8	0.25280200	-3.89564200	0.00000000
47	0.00000000	1.28185600	0.00000000

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CO<sub>2</sub>\_Ag<sub>20</sub>  
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47	-0.22616900	2.34103700	-0.09417800
47	-0.59756400	-0.66257600	0.16119400
47	-1.02549800	-3.55654400	0.60254300
47	1.77114500	-2.49114500	0.14831600
47	0.26757900	-1.77866500	2.79126300
47	1.36763200	0.60010400	4.29275100
47	-0.21205800	-2.40443500	-2.23675000
47	2.79612800	-2.52449800	-2.63546600
47	-2.76254900	-1.35010400	2.03414800
47	2.02631600	0.24469200	1.42576500
47	-0.98152100	1.07227600	2.54949300
47	1.38350000	2.99101700	2.29094400
47	-2.32343900	3.23771800	-1.96253000
47	0.59843800	2.66764500	-2.91088700
47	-1.46384800	0.44988100	-2.46038600
47	1.50595100	0.03941600	-1.93542200
47	-3.02415500	-1.79229400	-1.09387400
47	4.04673300	-0.59110300	-0.56369800
47	-2.97263500	1.16749400	0.17264300
47	2.71422100	2.36413400	-0.54773600
6	-6.17494100	-0.05230200	-0.05956400
8	-6.75171200	-1.02878700	-0.38806100
8	-5.58531100	0.92672600	0.26747500

CO<sub>2</sub>\_Ag<sub>21</sub>

47	4.95395800	-1.37767500	-0.69600800
47	1.68525800	0.91849300	2.63223800
47	3.51939200	-1.32106500	1.96431000
47	-2.24406500	-2.43759600	2.38198000
47	2.01150700	-2.20596900	-0.54790000
47	-2.74747900	-1.61107500	-2.42087400
47	-0.88348500	-2.77600100	-0.32647300
47	0.10246100	-1.05209400	-2.81112400
47	0.07451000	0.11409400	0.02802000
47	0.65999100	-1.93892500	2.25958200
47	-1.31297500	0.33913900	2.87380500
47	3.04336100	0.82165900	-0.13363100
47	-0.78744300	3.96300200	-1.66181900
47	-1.88210700	2.42391700	0.67095300
47	1.13494800	1.78431300	-2.39875800
47	1.10788100	2.99253200	0.44372700
47	-1.87366500	1.21964600	-2.19838200
47	2.99612200	-0.49749100	-2.85398100
47	-0.27348000	3.14073700	3.10209600
47	-3.92218200	-3.08241600	-0.06715200
47	-2.92474100	-0.32532500	0.32648400
6	-5.20913600	1.93912300	-1.20961500
8	-4.57615500	1.95553600	-2.21504600
8	-5.83888200	1.92520300	-0.20941100

CO<sub>2</sub>\_Ag<sub>22</sub>

47	1.49596000	-2.57170600	-1.29891700
47	-0.73816600	-0.94107000	-0.06926200
47	4.50517100	1.40635200	-0.25217600
47	1.37834900	-1.97395300	1.84956500
47	4.10851800	-1.46610900	0.05984000
47	-0.73572300	-3.77815000	0.53986100
47	3.03065000	0.47473300	2.49733900
47	-1.51889200	-1.67717700	2.69771300
47	-3.48494600	-1.90662800	0.12424300
47	-2.78079300	0.79355900	1.23889700
47	-2.70767100	0.23750200	-2.01462800

47	-3.36781600	2.91192900	-0.78508000
47	-1.48279700	-2.58547900	-2.38941300
47	-5.27656000	0.40733200	-0.42375000
47	-0.55598500	1.99285100	-0.84383000
47	0.18925600	-0.11301200	-2.94378000
47	1.84413100	0.26819000	-0.25551600
47	3.15479800	-0.48340200	-2.83710900
47	0.08711200	0.85907000	2.35602500
47	2.10892500	2.30013600	-2.31399800
47	-1.33704700	3.39782500	1.62240200
47	1.73424200	2.95452400	0.89618700
6	0.74681100	-1.08184600	5.44360900
8	1.84588000	-0.67121900	5.59435200
8	-0.35394400	-1.49788200	5.27708800

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CO<sub>2</sub>\_Ag<sub>2</sub>  
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47	-0.38129800	-0.09241900	-0.00199400
47	2.28252200	0.06822400	0.00092100
6	-4.06444900	0.05188500	0.00233800
8	-5.22072900	0.28632800	-0.00151200
8	-2.90062600	-0.18309800	0.00606300

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CO<sub>2</sub>\_Ag<sub>3</sub>  
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47	0.96519400	1.80025900	0.00001800
47	-0.76718800	-0.38036600	-0.00015300
47	1.83588300	-1.30499700	0.00009800
6	-4.34806900	-0.24372400	0.00007900
8	-5.47605200	0.09856000	0.00048300
8	-3.21199400	-0.59078000	-0.00032800

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CO<sub>2</sub>\_Ag<sub>4</sub>  
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47	-1.63040400	-1.82365200	-0.00016600
47	1.20912800	-1.37649400	0.00041100
47	-0.40134800	0.84562500	-0.00063700
47	2.45949700	1.22334100	0.00014300
6	-3.50079200	2.41477000	0.00050500
8	-4.67763300	2.47362000	0.00179800
8	-2.31339900	2.36098200	-0.00071400

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CO<sub>2</sub>\_Ag<sub>5</sub>  
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47	-0.14794100	-1.08142100	-0.00883500
47	-1.51633600	1.51612400	-0.24672200
47	1.37600600	1.40979000	-0.55528000
47	-2.98843200	-0.91132000	0.00062600
47	2.66775900	-1.13305900	-0.50064900
6	1.30245400	0.42760700	2.79945700
8	0.46492000	-0.41130200	2.72772700
8	2.13578200	1.26492700	2.87398600

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CO<sub>2</sub>\_Ag<sub>6</sub>  
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47	0.86249400	-1.52140600	-0.03241800
47	3.35922100	-0.18549100	-0.02561800
47	1.04454800	1.44365800	-0.07054300
47	-1.37338700	2.91732200	-0.25849000
47	-1.60767900	0.11197100	-0.54707100
47	-1.69450800	-2.71197800	-0.37279900
6	-1.26301700	-0.11506000	2.79022200
8	-0.08464000	-0.23987100	2.71975000
8	-2.43839800	0.00846400	2.86585200

CO<sub>2</sub>\_Ag<sub>7</sub>

47	-0.49457000	-2.37953000	-0.36985300
47	2.18074400	-1.47708200	0.54029300
47	2.19057200	1.46179300	0.54583700
47	0.76700200	0.00137500	-1.64357400
47	-0.26913900	-0.00094700	1.40102400
47	-0.47861400	2.38568600	-0.36099600
47	-2.11524800	0.01001300	-1.00729100
6	-3.80762300	-0.00278000	1.91482200
8	-3.31141100	-0.00967300	2.98860900
8	-4.29476000	0.00407500	0.83080600

CO<sub>2</sub>\_Ag<sub>8</sub>

47	1.77432500	1.58315900	-0.18803900
47	-0.13478500	0.47243100	1.95369600
47	-0.98646900	2.39470500	-0.14813800
47	-2.34751300	-0.35864100	0.14673600
47	-0.29273600	0.13646500	-1.95218700
47	0.03571800	-1.97364300	0.18844100
47	2.43176000	-0.75418100	1.51960600
47	2.30668700	-1.01651100	-1.52208100
6	-5.95644800	-1.03445100	0.00413000
8	-4.89126500	-0.52480500	0.12715900
8	-7.01494100	-1.54158600	-0.11871500

CO<sub>2</sub>\_Ag<sub>9</sub>

47	2.44160700	-1.70143900	-0.89657800
47	1.33931800	-0.91687300	1.74834500
47	-0.41609200	-1.74296300	-0.65788500
47	3.11058500	1.01953200	0.24229200
47	0.92265200	0.73635600	-1.82574700
47	-1.85350800	0.85539300	-1.00718500
47	0.30772200	1.80084400	0.90283600
47	-1.49453600	-0.38274400	1.82071000
47	-3.33143700	-1.58760400	-0.20281300
6	-2.19289500	4.10561300	-0.26491000
8	-2.89513800	3.32476700	-0.82335300
8	-1.48976500	4.87307600	0.29367600

CO<sub>2</sub>

6	0.00000000	0.00000000	0.00000000
8	0.00000000	0.00000000	1.18538400
8	0.00000000	0.00000000	-1.18538400

CO\_Ag<sub>10</sub>

47	-0.84442000	1.50770600	1.36041000
47	2.05517100	1.10799900	0.19551400
47	-1.64286000	-1.27797000	0.60533100
47	0.71543600	-0.75218000	2.34016200
47	1.27515200	-1.62125800	-0.48055200
47	-0.97670600	-2.07413500	-2.20982600
47	-3.38646300	0.98869100	-0.06432600
47	-0.69314500	0.71334000	-1.45175900
47	0.47838200	3.30424100	-0.70136300
47	4.04025300	-0.91035200	-0.12669700
6	-3.03577800	-2.88872300	1.46756500
8	-3.72037000	-3.62668600	2.03133200

CO\_Ag<sub>11</sub>

47	0.13240600	2.60302800	-0.00097700
47	1.45586300	0.39202500	1.52138900
47	4.00037800	0.42007000	0.00050500
47	1.45692200	0.39022700	-1.52202800
47	-1.48390600	0.68501900	-1.53929600
47	-0.27349000	-2.05027600	-1.47064100
47	2.39087000	-2.06497100	0.00180300
47	-0.27477000	-2.04690200	1.47074600
47	-1.48601200	0.68790400	1.54023300
47	-2.89474100	-1.47166200	0.00079800
47	-3.93794400	1.29527300	-0.00184300
6	3.68868000	3.65715500	-0.00190900
8	2.60572500	4.07369300	-0.00261600

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CO\_Ag12  
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47	0.80141400	0.36370700	-1.14377500
47	-2.14688100	0.27066700	-1.60851800
47	-0.69571700	-2.23526800	-0.99450700
47	1.41241800	-1.62334000	1.16092600
47	1.17384000	1.24540900	1.77123500
47	-1.26046500	-0.31203800	1.31012700
47	-3.69420900	1.25845900	0.67349800
47	-1.02164200	2.48221900	-0.04837300
47	-3.51415900	-1.78423700	-0.01498700
47	2.08539700	2.94814300	-0.50378100
47	3.56632500	0.42227300	0.01710300
47	2.61956500	-1.90504200	-1.51533000
6	2.07363800	-3.39002800	2.52734300
8	2.40518900	-4.10181700	3.37074800

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CO\_Ag13  
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47	1.42770000	-0.15460800	1.13791000
47	3.68554100	-1.61334200	-0.08728900
47	1.60180000	2.82830100	1.53773800
47	1.74459300	-0.37822600	-1.95655700
47	3.46563400	1.44098200	-0.33155000
47	0.82125900	-2.76565300	-0.31620100
47	-1.08273900	-0.52743900	-1.08626300
47	-1.13420000	1.28865200	1.54507300
47	0.39046800	2.03776500	-0.99832900
47	-3.54330500	-0.56078500	0.57022700
47	-1.03035000	-1.63624200	1.82298600
47	-2.73485800	1.94898500	-0.80574800
47	-2.24456200	-3.15043800	-0.43813600
6	-4.97974500	4.69300000	-2.09249900
8	-4.29621000	3.77728700	-1.91955800

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CO\_Ag14  
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47	0.64199000	1.13528900	1.10961500
47	0.00463500	-1.71929400	1.26725700
47	2.97794300	-0.82370400	1.44247300
47	-2.16371600	0.27633400	1.50007200
47	-1.07815600	-0.20257500	-1.27755000
47	-2.91213200	-2.17181500	-0.11956700
47	-3.87573300	0.69532600	-0.86992300
47	2.25683100	-3.46878700	0.21924300
47	1.79927400	-0.87768000	-1.26034600
47	3.29790400	1.74845000	-0.02038400
47	-0.31621100	-3.21465400	-1.22161400
47	0.93767200	1.82193800	-1.87396500
47	-1.59192500	2.65812800	-0.30804500
47	1.12591800	3.93039100	0.23431200

6	-3.39617600	0.61322200	3.38435200
8	-3.94060400	0.78941900	4.38496500

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CO\_Ag15  
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47	-0.02167600	4.00540700	-0.05884000
47	0.39123400	-1.46285200	1.44094700
47	0.39071000	1.46270500	1.44120300
47	-2.07357100	-0.00043300	2.16806300
47	-2.36159800	2.21848700	0.16327600
47	2.97072200	0.00024700	1.17754100
47	0.10100200	1.46892300	-1.62086700
47	0.10133400	-1.46829700	-1.62134500
47	-2.43660700	-0.00009900	-1.86823300
47	2.70906400	0.00039100	-1.78770800
47	2.63546000	2.62820200	-0.30459900
47	2.63613800	-2.62743400	-0.30574300
47	-2.36079100	-2.21905600	0.16323600
47	-4.40855100	-0.00087800	0.33453500
47	-0.02038400	-4.00528200	-0.05857200
6	6.51570100	0.00003000	2.59336800
8	5.37986900	-0.00021600	2.38546600

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CO\_Ag16  
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47	1.34304500	-3.33539600	-0.43127600
47	-1.56806800	0.98815800	2.44591300
47	-0.05551200	-1.37343200	1.50071200
47	1.31804200	1.17370700	1.55340500
47	2.89934500	-1.25807200	1.19053700
47	-3.13772700	-1.24916500	1.58451700
47	-0.29220000	-1.09575500	-1.74276000
47	-1.89374600	1.34286500	-2.10391400
47	1.08666400	1.45691400	-1.70529200
47	-3.37557900	-0.99716200	-1.34444700
47	-1.67456700	-3.25726500	-0.17956300
47	-3.61077000	1.51673900	0.32878200
47	1.91251100	3.69860800	0.08545100
47	3.69480800	1.26117900	-0.22912200
47	-0.96821600	2.98822300	0.25903200
47	2.68232000	-1.01664700	-1.87077800
6	6.08525600	-3.14371500	2.24057800
8	5.06899000	-2.59778300	2.19003300

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CO\_Ag17  
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47	-2.44577600	-2.17109900	-1.41361300
47	3.03938200	1.74858100	-0.90886500
47	-1.67250300	3.49037200	-0.16394800
47	-0.95946300	-0.34277600	-3.22565200
47	-1.70797600	1.41457600	1.95089600
47	3.40622200	-1.26552800	-0.78489400
47	0.56787300	-2.10658800	-1.35946600
47	-2.98824300	-1.16521300	1.37818000
47	1.83034200	-2.72784700	1.27257200
47	-1.01451700	-3.39229100	0.93312200
47	0.73210800	1.46928500	3.62017000
47	1.96506900	-0.00106400	-3.09374600
47	0.97695900	2.75508300	0.94041800
47	-0.29706600	-1.14642100	2.69441200
47	2.38036300	0.19263100	1.55444500
47	-2.44429600	0.73307100	-0.85961600
47	0.24129300	2.06953200	-1.90676000
6	-6.02762300	1.39991900	-2.29968100
8	-4.93669000	1.56852300	-1.96271300

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CO_Ag18			
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47	3.25503900	0.04435300	-1.18777600
47	-2.40752600	-0.11670100	3.30522800
47	-0.50244100	3.47827400	0.18894100
47	0.66279900	0.11521200	-3.31557800
47	2.31467200	2.48005600	0.66669200
47	-0.00241800	1.47262500	2.39574800
47	-1.52770100	1.64213400	-1.92570000
47	-2.66335100	-1.63764800	0.80895400
47	-1.52529100	-1.50769800	-2.03449600
47	2.31883100	-2.51705300	0.49533900
47	1.33397200	-2.48753100	-2.24523000
47	2.56626300	-0.06754600	2.03228300
47	-0.49643300	-3.48412700	-0.05055800
47	-3.95191200	0.04025400	-1.24268200
47	1.32926500	2.63984900	-2.06928500
47	0.00117200	-1.63324600	2.28961400
47	-2.66668800	1.57305900	0.92128300
47	0.54743000	0.00799400	-0.22548400
6	4.27493100	-0.12347000	3.54653300
8	5.10291800	-0.15568000	4.34725300

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CO_Ag19			
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47	2.81859400	0.11572800	2.53530600
47	-2.41110500	1.15401000	-2.36747600
47	-4.00990600	-0.26240400	-0.06924700
47	-2.28432400	-1.96286600	-2.18306900
47	2.49326300	2.62202600	0.52515600
47	-2.21706600	-2.74796700	0.87922300
47	-1.11249900	-0.21915700	-0.11928500
47	2.85983700	-2.66767500	0.82646900
47	0.34209700	-1.63450300	2.13407200
47	0.11074600	2.37408400	-1.30598000
47	-2.30192300	-0.13435600	2.56858500
47	2.74251800	-1.84368100	-2.37575400
47	2.66958900	1.39835000	-2.46210300
47	0.19791300	-0.35388900	-2.87281900
47	-2.34855100	2.33835300	0.58090200
47	0.33778900	-2.76535900	-0.80736100
47	-0.04311500	4.21347100	1.04263500
47	0.19985300	1.47078500	2.14825400
47	1.83666300	-0.13802300	-0.17335700
6	0.24883200	-3.42880800	5.62574000
8	0.51618400	-3.05034300	4.56879700

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CO_Ag1			
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6	0.42886000	-1.80247100	0.00000000
8	-0.32164500	-2.69096900	0.00000000
47	0.00000000	0.68814000	0.00000000

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CO_Ag20			
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47	0.77538700	-1.25475700	-1.82206500
47	-0.83416500	0.58218100	0.03273900
47	-2.21047500	2.48781300	1.75663500
47	0.45523100	1.27252000	2.65360100
47	0.43847000	3.28170800	0.27218200
47	2.94007800	3.18724700	-1.43327600
47	-2.02267700	-0.59618800	2.46977900
47	0.29169700	-1.16652700	4.32484200
47	-2.19191200	2.70205600	-1.43352100

47	2.18873300	0.85962400	0.23050600
47	0.55196400	1.68899000	-2.38253400
47	3.26506500	0.25772300	-2.42957300
47	-1.25690400	-3.09290600	-2.94962700
47	0.57181000	-3.90012300	-0.54728000
47	-1.93356100	-2.16437900	-0.21461200
47	0.58404500	-1.73777100	1.44708200
47	-3.74044400	0.29357900	0.00425800
47	2.95599900	-0.52332700	2.72269800
47	-1.96095100	-0.18922200	-2.59279700
47	3.13228500	-1.92637500	-0.09761600
6	-6.11214400	0.05982500	-0.01878400
8	-7.16399500	-0.40833000	-0.05302200

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CO\_Ag21  
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47	-4.83488400	-1.32133100	-0.00150600
47	-1.26827000	1.47146400	-2.56675800
47	-3.11411000	-0.86098500	-2.44798500
47	2.67364700	-1.87966200	-2.45409100
47	-1.86878200	-2.16542900	-0.00202300
47	2.67327600	-1.88333200	2.45234600
47	1.05823700	-2.66538000	-0.00194600
47	-0.23122500	-1.42539700	2.58051800
47	0.06467000	0.22319600	-0.00047600
47	-0.23060500	-1.42140800	-2.58388700
47	1.74719100	0.93421000	-2.56623500
47	-2.90364300	0.91642900	0.00032600
47	0.69799700	3.73750900	2.42811300
47	2.04791000	2.62044900	0.00219900
47	-1.26887600	1.46755000	2.56796100
47	-0.95350400	3.14063400	0.00206900
47	1.74616100	0.93017400	2.56795300
47	-3.11448400	-0.86496200	2.44651000
47	0.69851800	3.74125500	-2.42248400
47	4.09839200	-2.94313500	-0.00178500
47	3.10979100	-0.14608100	0.00047200
6	-2.73456100	-6.04866900	0.00651800
8	-2.81009100	-4.89738200	-0.00072500

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CO\_Ag22  
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47	1.44338900	2.57872200	1.14583700
47	-0.74797700	0.89889300	-0.01027300
47	4.54124600	-1.36835300	0.08792400
47	1.26612700	1.98567800	-1.97861300
47	4.12291900	1.50503400	-0.24955100
47	-0.87553100	3.72606200	-0.59591700
47	3.03215200	-0.43317400	-2.62896600
47	-1.59894600	1.59472500	-2.75417700
47	-3.54913800	1.68350500	-0.09078200
47	-2.73640900	-0.96357700	-1.24990000
47	-2.61187900	-0.42440100	1.98820800
47	-3.18752300	-3.13434300	0.76250100
47	-1.48510200	2.47807700	2.32991600
47	-5.21371100	-0.72516900	0.45527800
47	-0.43999900	-2.03572500	0.71899700
47	0.27492400	0.04886300	2.84788200
47	1.86957300	-0.24662500	0.10481800
47	3.20804800	0.55283400	2.64384600
47	0.09031500	-0.90473100	-2.46707400
47	2.27057900	-2.32418200	2.10020600
47	-1.22472000	-3.51774800	-1.69087500
47	1.85641400	-2.94360900	-1.04966500
6	-1.15464900	6.01991300	-1.15026500

8 -0.92442400 7.05437500 -1.60256500

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CO\_Ag2

-----  
6 4.51339500 0.04373600 -0.00343600  
8 3.35810800 -0.00664100 0.00936900  
47 0.75994500 -0.01120800 -0.00209200  
47 -1.90771600 0.00675500 0.00093600

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CO\_Ag3

-----  
47 -1.93058700 -0.00233100 0.00027400  
47 0.49290400 1.47277100 -0.00025200  
47 0.49791700 -1.47105400 -0.00025200  
6 2.48170100 0.00145900 0.00041300  
8 3.65985400 0.00251500 0.00104200

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CO\_Ag4

-----  
47 -2.53226100 -0.30835900 0.00002500  
47 0.00024100 1.09350600 -0.00122900  
47 -0.00074100 -1.65718100 0.00064800  
47 2.53167300 -0.31079600 0.00002400  
6 0.00247300 3.31196900 -0.00038500  
8 0.00454000 4.46514400 0.00341600

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CO\_Ag5

-----  
47 -0.21015500 -1.00325600 -0.00043200  
47 0.94430100 1.66738000 -0.00036800  
47 -1.96833800 1.40598400 0.00041900  
47 2.60977500 -0.66205400 -0.00087000  
47 -3.05162400 -1.22149800 0.00044500  
6 5.01101400 -0.85938500 0.00146300  
8 6.08848400 -0.45148000 0.00363900

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CO\_Ag6

-----  
47 -1.11814400 1.43369000 -0.03731400  
47 -3.46214200 -0.12525300 0.35013400  
47 -1.00863300 -1.49999100 -0.04399900  
47 1.48644400 -2.72747500 -0.48597300  
47 1.56149600 0.07021900 0.16426900  
47 1.27526200 2.85677000 -0.45153800  
6 3.61559600 0.03140100 1.52083600  
8 4.72438900 -0.07031500 1.82284500

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CO\_Ag7

-----  
47 2.13414300 1.67147700 -0.01426800  
47 2.45914400 -1.20540900 -0.02124000  
47 -0.27530400 -2.45572700 0.00826000  
47 0.20625700 -0.00724000 1.57408300  
47 0.17527700 -0.00593000 -1.56930700  
47 -2.31681800 -0.29369200 0.02845100  
47 -0.80685400 2.28027100 0.01416800  
6 -4.67323100 -0.17068400 -0.02327200  
8 -5.75316200 0.22348300 -0.10090900

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CO\_Ag8

-----  
47 0.33341700 0.38331700 1.94285000  
47 -0.00738800 -1.98845700 0.15095400  
47 -2.33727200 -0.62537600 1.51104500  
47 -2.25147700 -0.84187000 -1.51489300



47	-1.53442100	1.68185800	-0.15283000
47	0.44062700	0.11242200	-1.93473000
47	2.49554000	-0.53798300	0.12084800
47	1.28842200	2.29705200	-0.11281400
6	4.76391100	-1.21209400	0.04198300
8	5.66580900	-1.91659100	-0.09275900

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CO\_Ag<sub>9</sub>  
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47	-2.29525300	-1.58198100	-0.00305400
47	-0.83313200	0.18209800	-1.92021600
47	0.57739500	-1.65115300	-0.00192200
47	-2.73547600	1.47121200	0.00011700
47	-0.83496000	0.17784600	1.91957200
47	1.99842400	0.61791100	1.52989900
47	0.13599400	2.34538600	0.00249800
47	2.00004400	0.62200800	-1.52713200
47	3.51827400	-1.43073300	-0.00051500
6	-4.48971400	-2.43097300	0.00027900
8	-5.62915400	-2.59825700	0.00420900

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CO  
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6	0.00000000	0.00000000	-0.66158900
8	0.00000000	0.00000000	0.49619200

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H<sub>2</sub>O\_Ag<sub>10</sub>  
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47	1.33277500	-1.49961300	-1.01944100
47	1.36778300	1.46191800	-1.02757800
47	-1.58572100	-1.46471800	-0.24435300
47	-0.54427100	0.00378000	-2.73941900
47	-1.55537300	1.46952800	-0.21745300
47	-3.95131200	0.01705000	0.43192900
47	0.29637900	-3.03964000	1.23656300
47	0.92761300	-0.01974800	1.56082400
47	3.58243800	-0.03605500	0.19618100
47	0.35970100	3.07907100	1.18284900
8	-0.97460700	0.10216100	3.02354500
1	-1.31995900	1.00461100	3.18183000
1	-1.69376600	-0.48575100	2.70502300

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H<sub>2</sub>O\_Ag<sub>11</sub>  
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47	0.09658200	-2.63088300	-0.37755900
47	1.66851200	-0.42131700	-1.62994000
47	4.02099100	-1.02360700	0.03863200
47	1.43151100	-0.81671900	1.47456000
47	-1.58383300	-0.87530200	1.36881200
47	-0.03401700	1.73090200	1.61501100
47	2.72909200	1.62127700	0.32715000
47	0.20289200	2.14304900	-1.31136500
47	-1.29547900	-0.39995500	-1.66952900
47	-2.57554500	1.73115500	0.02291400
47	-3.98079100	-0.78281500	-0.54083400
8	-3.12057200	-1.30839100	3.12971300
1	-2.92026000	-1.28647800	4.08211500
1	-4.07108900	-1.20830900	2.94107300

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H<sub>2</sub>O\_Ag<sub>12</sub>  
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47	1.03827400	0.00049200	-1.18292900
47	-1.85205200	0.00011600	-1.75524900
47	-0.71356200	-2.37608700	-0.48786800
47	1.28833300	-1.44412400	1.63647900

47	1.28835100	1.44380900	1.63604800
47	-1.32305600	0.00024000	1.38802900
47	-3.58226700	1.57043300	-0.02593400
47	-0.71341900	2.37643100	-0.48763500
47	-3.58230300	-1.57010800	-0.02586400
47	2.56161100	2.48635900	-0.81915300
47	3.68494300	-0.00074600	0.26739300
47	2.55973400	-2.48669300	-0.81982400
8	-2.99342000	-0.00051800	3.11142200
1	-3.92657600	0.00020600	2.82428500
1	-2.89166900	-0.00181400	4.08024300

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H<sub>2</sub>O\_Ag<sub>13</sub>  
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47	-1.17946900	0.28371500	1.07795700
47	-2.95463700	2.51039100	0.34374200
47	-2.30045600	-2.51647100	1.05148000
47	-1.46263300	1.21119200	-1.87151900
47	-3.62534300	-0.38635000	-0.47929700
47	0.13873900	2.83691400	0.16590200
47	1.26019300	0.33579600	-1.20396900
47	0.87258200	-1.89531500	1.04579800
47	-0.94489200	-1.68864600	-1.40974900
47	3.66053500	-0.68356600	0.24369400
47	1.60114000	0.78069400	1.90187100
47	2.08093400	-2.55040000	-1.51139000
47	3.16228900	2.31484400	-0.08040700
8	-1.49214500	-2.62864500	3.31594800
1	-0.87674100	-1.87397600	3.43487400
1	-1.70831600	-3.07822900	4.15418400

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H<sub>2</sub>O\_Ag<sub>14</sub>  
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47	-1.68296000	-0.62085800	1.32081600
47	-0.32659700	1.94504500	1.74517500
47	-2.80986400	2.41750600	0.04630700
47	1.24755100	-0.41894700	1.17488400
47	2.12747400	-0.02829300	-1.76427400
47	4.10037700	0.01584100	0.48968100
47	2.64453600	-2.59304500	-0.22764200
47	-0.25188100	4.10396200	-0.31420100
47	-0.41232200	1.27694400	-1.20282200
47	-3.11015400	-0.23685700	-1.24027900
47	2.18614800	2.34457100	0.11883900
47	-0.28110900	-1.62458900	-1.39472100
47	0.01838800	-3.29363400	0.96286700
47	-2.69066000	-3.04909700	-0.32543300
8	-3.47410000	-1.11910900	2.81587800
1	-4.30970000	-1.46142300	2.45073600
1	-3.56703200	-0.79748600	3.73004200

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H<sub>2</sub>O\_Ag<sub>15</sub>  
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47	-0.13745200	3.99229900	-0.06915300
47	-0.51661500	-1.46737100	-1.61402800
47	-0.51797300	1.47020200	-1.61302400
47	1.95572100	0.00286900	-2.29721100
47	2.16863000	2.14192000	-0.18369700
47	-3.09545400	-0.00015000	-1.31518600
47	-0.30983100	1.45261400	1.47412900
47	-0.31092400	-1.45320800	1.47265300
47	2.22787400	-0.00066000	1.97025300
47	-2.92219300	-0.00049900	1.66675400
47	-2.80241000	2.62604000	0.13985900
47	-2.80392800	-2.62713300	0.13823100

47	2.16793400	-2.14131100	-0.18843600
47	4.22661400	0.00018000	-0.33524400
47	-0.13816100	-3.99115900	-0.07278000
8	3.72473600	-0.02006100	3.80763100
1	4.68499500	-0.02748000	3.64745400
1	3.50097600	-0.02980300	4.75485100

H<sub>2</sub>O\_Ag<sub>16</sub>

47	0.59991800	3.67813200	0.24354700
47	-1.36934100	-1.16930900	-2.46388800
47	-0.41197700	1.42861900	-1.50952200
47	1.51695700	-0.70598300	-1.75747700
47	2.52002700	2.06339900	-1.47396400
47	-3.43771400	0.57561800	-1.44123100
47	-0.37248500	1.09879200	1.74349200
47	-1.30047600	-1.73298200	2.18425600
47	1.61637300	-1.02976900	1.54484400
47	-3.23820400	0.24495900	1.50679500
47	-2.33061900	2.86615100	0.22957400
47	-3.04610000	-2.20645200	-0.21103500
47	2.80978900	-3.00441500	-0.34469600
47	3.96378400	-0.18810000	-0.13157600
47	-0.15965700	-2.99204000	-0.39492000
47	2.49846900	1.74586600	1.61412100
8	0.61057900	-3.07694800	3.06572100
1	0.92321800	-3.09334100	3.99044200
1	0.83108500	-3.89795200	2.58275900

H<sub>2</sub>O\_Ag<sub>17</sub>

47	-2.63583000	2.55466800	0.08495300
47	3.60100400	-0.37618500	0.11965400
47	0.00551100	-1.36281400	3.61636000
47	0.01845100	3.19213200	1.40271000
47	-1.68287200	-2.28552500	1.37017000
47	2.65985500	0.91604700	-2.45723600
47	0.00304700	1.29828500	-0.81007000
47	-3.60199900	-0.34862500	0.14187400
47	-0.01187800	0.09610200	-3.49497000
47	-2.67059200	0.93500600	-2.44214400
47	-0.01595600	-3.94042200	-0.43272200
47	2.65792800	2.53436100	0.07055700
47	1.67404000	-2.29795700	1.36079400
47	-1.54081900	-1.63508600	-1.54375200
47	1.51644900	-1.64428500	-1.55095200
47	-1.50322100	0.63145800	1.99365200
47	1.52326600	0.62026800	1.98697900
8	0.01728100	5.13971600	2.68528400
1	-0.79419300	5.58547600	2.98403500
1	0.82592700	5.58766400	2.98839700

H<sub>2</sub>O\_Ag<sub>18</sub>

47	-1.21666700	3.89804100	-0.04363300
47	3.07773100	-1.76454600	-0.09769900
47	-0.34502300	0.00227000	3.11728900
47	-4.14250800	0.00149800	0.02207800
47	0.73110800	2.45422100	1.66930200
47	2.49252400	0.00036500	2.22893600
47	-2.21595300	-1.61275500	1.59666900
47	0.77878300	-2.53656700	-1.87661800
47	-2.07287100	-1.50758200	-1.48927500
47	0.78037900	2.53323100	-1.87931600
47	-2.07073200	1.50705000	-1.48993800

47	3.07949000	1.76183700	-0.09919600
47	-0.19935300	-0.00244000	-3.18449500
47	-1.22042600	-3.89673000	-0.03982200
47	-2.21527700	1.61718800	1.59566000
47	2.63571900	-0.00144700	-2.48485800
47	0.72886100	-2.45245600	1.67240100
47	0.58061000	-0.00068500	-0.13044700
8	3.77025000	-0.00218800	4.19752100
1	4.03744300	-0.81304700	4.66412200
1	4.03996400	0.80734000	4.66498900

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H<sub>2</sub>O\_Ag<sub>19</sub>  
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47	-2.69513500	0.89808800	-2.58070500
47	2.36874500	0.46031700	2.54172900
47	3.99071400	-0.39384800	0.00012300
47	2.18030100	-2.49526000	1.58030700
47	-2.37905100	2.79707300	-0.00002200
47	2.18046300	-2.49631900	-1.57781000
47	1.09236800	-0.28316900	0.00016400
47	-2.92639000	-2.21047800	-1.64418200
47	-0.31680900	-1.03999500	-2.56740600
47	-0.07234000	2.01770700	1.77551300
47	2.36890400	0.45827000	-2.54189100
47	-2.92695000	-2.20925300	1.64415600
47	-2.69650400	0.89683700	2.57978900
47	-0.31732900	-1.03891100	2.56778900
47	2.42078200	2.34401100	-0.00132200
47	-0.45448700	-2.89648800	0.00115000
47	0.21627100	4.39967300	0.00009100
47	-0.07148100	2.01752200	-1.77588300
47	-1.83467500	-0.07989300	-0.00048600
8	-0.56714300	-5.28242100	-0.00650400
1	-0.78125900	-5.79183700	-0.80798500
1	-0.66929100	-5.80537900	0.80820000

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H<sub>2</sub>O\_Ag<sub>1</sub>  
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47	-0.44647800	0.00000100	-0.00000300
8	1.99036800	0.00001300	0.00010800
1	2.53090900	0.81066800	-0.00035200
1	2.53062100	-0.81083200	-0.00035200

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H<sub>2</sub>O\_Ag<sub>20</sub>  
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47	-0.22206700	2.58551200	-1.38967300
47	-0.05522100	-0.00127300	0.53346500
47	0.42784200	-1.71229300	3.24258100
47	1.03170900	-2.79334800	0.48034800
47	2.75734900	-0.52372100	1.71098000
47	4.55386400	1.04409300	-0.16218500
47	-1.88179900	-2.28500300	1.32642800
47	-1.17349600	-4.36380900	-0.77299000
47	0.90634200	1.26271100	3.34697400
47	2.55116400	-0.83201400	-1.24490700
47	1.93507500	2.23603900	0.68070200
47	2.54337400	1.99759500	-2.25390500
47	-3.01019900	3.32781700	-0.70961500
47	-2.51746000	1.07362000	-2.63696300
47	-3.01798600	0.45963400	0.32788200
47	-1.77235000	-1.58185200	-1.59093300
47	-1.89842800	0.18754600	3.12786200
47	0.79361300	-2.85296500	-2.52559000
47	-1.08903200	2.63893000	1.49332300
47	0.30516000	0.09633700	-3.00490800

8	-5.38733800	0.17570000	0.14115500
1	-6.01290300	0.92181000	0.15357600
1	-5.75867900	-0.61456000	-0.28999700

H<sub>2</sub>O\_Ag<sub>21</sub>

47	-4.49350200	-2.22218000	0.69952800
47	-1.72374500	0.59052400	-2.66883900
47	-3.11008500	-1.94539300	-2.02541200
47	2.76469500	-1.94495200	-2.32242800
47	-1.48408700	-2.48474000	0.52443300
47	3.07359100	-1.07491700	2.49474400
47	1.46181700	-2.51831500	0.38201600
47	0.17182300	-0.98603000	2.82877400
47	-0.01033400	0.14653100	-0.02589300
47	-0.18462800	-2.00648700	-2.26680100
47	1.32690900	0.56840300	-2.89922300
47	-3.06991200	0.28825700	0.06770100
47	0.03686200	4.15390400	1.54860000
47	1.47026100	2.75757600	-0.70832100
47	-1.37891900	1.64106600	2.34465800
47	-1.58870800	2.77258700	-0.51766500
47	1.79032400	1.68293700	2.06952900
47	-2.75846300	-0.92583700	2.82198300
47	-0.18427600	3.14756200	-3.14281100
47	4.50266700	-2.30564900	0.09743600
47	3.02679100	0.24316100	-0.26826100
8	1.76895400	2.01164900	4.46327100
1	1.07200600	2.60491400	4.80744000
1	1.73963400	1.13557900	4.90024200

H<sub>2</sub>O\_Ag<sub>22</sub>

47	-1.55841000	-2.64987100	1.08576100
47	0.74199600	-1.03085500	-0.07667800
47	-4.42420500	1.41714900	0.22812400
47	-1.36560500	-2.00786700	-2.03595900
47	-4.19769600	-1.46957800	-0.37002300
47	0.69725000	-3.85086300	-0.70966600
47	-3.05601700	0.45803900	-2.62524100
47	1.52587700	-1.76806900	-2.83721700
47	3.52146200	-1.91168700	-0.12969300
47	2.80806100	0.73742800	-1.34083900
47	2.63629200	0.18407700	1.97073900
47	3.32601000	2.85127500	0.78162800
47	1.46362100	-2.70563100	2.21552400
47	5.25227500	0.46915000	0.42287600
47	0.55934700	1.87362300	0.62641700
47	-0.26094100	-0.27313300	2.77534400
47	-1.84775600	0.17718700	0.08019900
47	-3.23300600	-0.51795200	2.58666700
47	-0.05735800	0.77721700	-2.54432800
47	-2.10476900	2.30064300	2.10054200
47	1.35914600	3.32904000	-1.78564000
47	-1.74239000	2.86084500	-1.09749400
8	-0.31384300	3.51041400	3.19724000
1	0.35071200	2.89666900	3.57624600
1	0.13031200	4.26208700	2.75683800

H<sub>2</sub>O\_Ag<sub>2</sub>

47	-0.97367700	-0.00014700	-0.00006800
47	1.70063600	0.00006800	0.00003300
8	-3.30878400	0.00030000	0.00013200
1	-3.84785700	0.81032600	0.00029500

1 -3.84895500 -0.80899600 0.00029700

H<sub>2</sub>O\_Ag<sub>3</sub>

47 -1.03211800 1.55881000 0.00001600  
47 -1.02999400 -1.55986600 0.00000400  
47 1.27658200 0.00069500 -0.00003900  
8 3.58435900 0.00170700 0.00007300  
1 4.12245900 -0.80820800 0.00072900  
1 4.12257700 0.81154100 -0.00043400

H<sub>2</sub>O\_Ag<sub>4</sub>

47 2.54897200 -0.22766700 -0.00045700  
47 0.00025800 -1.53475000 0.00089500  
47 -0.00070300 1.21956600 -0.00044500  
47 -2.54887000 -0.22769000 -0.00046000  
8 0.00147000 3.51437000 0.00201100  
1 0.81305800 4.04919100 0.00266200  
1 -0.80870500 4.05131900 0.00319700

H<sub>2</sub>O\_Ag<sub>5</sub>

47 -0.00097900 0.93482500 -0.00003400  
47 1.43531000 -1.62693800 -0.00016800  
47 -1.43758500 -1.62502800 -0.00011900  
47 2.92535200 0.79591200 0.00030400  
47 -2.92533700 0.79962700 0.00028100  
8 0.01425200 3.28434800 -0.00115000  
1 0.83308800 3.81295200 -0.00142300  
1 -0.79491200 3.82755600 -0.00175200

H<sub>2</sub>O\_Ag<sub>6</sub>

47 -0.99380800 1.46196200 -0.00542900  
47 -3.42978300 -0.00038400 0.03824900  
47 -0.99334700 -1.46201800 -0.00525500  
47 1.43179200 -2.87767600 -0.05731100  
47 1.67010700 0.00020500 0.03120600  
47 1.43128700 2.87788200 -0.05721500  
8 4.04638600 0.00013900 0.25306300  
1 4.58270900 0.81171800 0.29767400  
1 4.58254800 -0.81151400 0.29827300

H<sub>2</sub>O\_Ag<sub>7</sub>

47 -2.22423300 -1.45082200 0.00085200  
47 0.61905000 -2.38011900 0.00047200  
47 2.41504400 -0.00061300 0.00078500  
47 -0.12190500 -0.00071900 -1.58383700  
47 -0.12305600 0.00011400 1.58296000  
47 0.62040100 2.37960000 0.00022100  
47 -2.22280400 1.45251500 -0.00118100  
8 4.76829300 0.00013600 -0.00122700  
1 5.30869100 -0.80650900 -0.06643700  
1 5.30763000 0.80748100 0.06343500

H<sub>2</sub>O\_Ag<sub>8</sub>

47 0.65894500 0.14081700 -1.88644700  
47 -1.21197600 1.66912600 0.00004400  
47 -1.99890100 -0.83193800 -1.52693500  
47 -1.99864600 -0.83203800 1.52706600  
47 0.18955100 -2.20717900 -0.00020900  
47 0.65933300 0.14039000 1.88646600

47	1.65251700	2.14789500	0.00006400
47	2.72924800	-0.90129000	-0.00016300
8	-3.10586900	3.11004300	0.00054300
1	-3.55593200	3.40722900	-0.80963100
1	-3.56038300	3.40060700	0.81065500

H<sub>2</sub>O\_Ag<sub>9</sub>

47	1.91597800	2.19219600	-0.10660100
47	1.08117000	0.01336500	-1.90899600
47	-0.94678900	1.52846800	-0.12148200
47	3.27064400	-0.60170700	0.04492800
47	1.05230200	0.21724700	1.89856600
47	-1.51910400	-0.96986200	1.58274200
47	0.79913900	-2.22068500	0.11720300
47	-1.49397700	-1.13795700	-1.50315400
47	-3.69463900	0.19640200	-0.04370300
8	-2.13251600	3.59081400	0.15294300
1	-3.09852400	3.63547100	0.27316600
1	-1.68343500	4.41713900	0.40670800

H<sub>2</sub>O

8	0.00000000	0.00000000	0.10951200
1	-0.00000000	0.80334700	-0.43804900
1	-0.00000000	-0.80334700	-0.43804900

NO<sub>2</sub>\_Ag<sub>10</sub>

47	2.40787100	-0.27541800	0.85040500
47	-0.12013400	-1.91322900	0.39857500
47	0.26300700	1.83466700	0.93289000
47	0.09868300	-0.32680100	2.90565700
47	-2.23377000	0.28188200	1.14523100
47	-1.69222100	2.08048400	-1.18420400
47	2.60695800	2.13408400	-0.77157400
47	0.59903500	0.09148000	-1.62418200
47	2.39613900	-2.44729100	-1.04118200
47	-2.12767000	-0.92724800	-1.57985000
7	-4.94582900	-1.22482900	-0.01483600
8	-4.28573300	-0.67470500	0.94877500
8	-4.29932300	-1.38266400	-1.12241100

NO<sub>2</sub>\_Ag<sub>11</sub>

47	-0.31776100	-2.56272500	0.98792500
47	-1.39318200	0.01817100	1.66380900
47	-4.16785600	-0.55171600	0.42291800
47	-1.88929500	-1.27462100	-1.26311300
47	1.06752400	-1.34008600	-1.30672700
47	-0.29552300	1.10007900	-2.14195300
47	-2.58643400	1.72427300	-0.30990800
47	0.13068700	2.36008600	0.58186700
47	1.57787200	-0.36753000	1.63176100
47	2.61272100	1.16904700	-0.90634700
47	3.83924200	-1.33035600	-0.35833600
7	2.73265900	1.71849400	2.07608800
8	2.48066800	2.58049700	1.06995100
8	3.48253500	2.11616800	2.97733400

NO<sub>2</sub>\_Ag<sub>12</sub>

47	-1.01347000	0.07832300	-1.09061000
47	1.77144200	-0.45401900	-1.65886700
47	0.89347600	2.19921300	-0.50490600

47	-1.12583700	1.45516400	1.68151200
47	-1.59900400	-1.40630700	1.67112400
47	1.14276500	-0.39941100	1.32278100
47	3.22537400	-2.22065300	0.24158000
47	0.15947000	-2.72306400	-0.45498000
47	3.78467700	0.61524800	0.25515800
47	-2.85402700	-2.15766000	-0.92376200
47	-3.72641600	0.42384600	0.19538900
47	-2.19144500	2.77306000	-0.75514500
7	2.73711700	3.49077800	-0.05700600
8	2.74801500	4.74078700	-0.06776800
8	3.86335600	2.87530600	0.23941800

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NO<sub>2</sub>\_Ag<sub>13</sub>  
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47	1.22148800	-0.58214300	1.09430800
47	3.12682500	-2.51513700	-0.06065900
47	2.20861700	2.07022400	1.75371100
47	1.54901900	-0.73397500	-1.92333100
47	3.74553600	0.41620800	-0.08560600
47	0.02548400	-2.83903500	-0.42475900
47	-1.21889300	-0.18096400	-1.13586300
47	-0.94639500	1.34078100	1.59265600
47	0.89736500	1.97225500	-0.91501700
47	-3.67294200	0.30006100	0.41745600
47	-1.52174700	-1.57749500	1.71397400
47	-2.34671400	2.61493000	-0.67808200
47	-3.06552600	-2.50392600	-0.60141800
7	0.18309400	4.11862600	-1.43058200
8	0.93811400	5.05942500	-1.75924200
8	-1.11075900	4.36880000	-1.37979100

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NO<sub>2</sub>\_Ag<sub>14</sub>  
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47	0.27332900	1.23342200	-1.20471100
47	-1.66131900	-0.99384800	-1.26408400
47	-2.70773800	1.91820800	-1.16923200
47	1.19952500	-1.47105900	-1.97369100
47	0.59190500	-1.12004000	0.99855200
47	-0.07813800	-3.71254800	-0.33425700
47	2.76400700	-2.97191400	0.03755900
47	-4.16167100	-0.35391800	0.19623600
47	-1.56927500	0.79419000	1.35516500
47	-0.65593100	3.55969100	0.31657600
47	-2.17754000	-2.23371700	1.35384200
47	1.29008500	1.68941800	1.68099700
47	3.03563100	0.44412000	-0.55839500
47	2.30281400	3.33191700	-0.61631600
7	3.49180600	-0.45171900	2.72383500
8	2.95803400	0.66639000	3.00987700
8	3.11823200	-0.94042900	1.54961400

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NO<sub>2</sub>\_Ag<sub>15</sub>  
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47	-3.79795400	-2.38779200	-0.25845700
47	0.40495200	1.58084300	-1.20580000
47	-1.74750100	-0.45147100	-1.39023900
47	-2.55548400	2.44138000	-1.07178100
47	-3.88913400	0.35816100	0.57564200
47	1.11105400	-1.27733700	-1.27261300
47	-1.31217200	-1.36957800	1.42237100
47	1.42003600	-0.13200500	1.39216100
47	-1.07312700	1.52554100	1.42173600
47	1.31711500	-3.11251200	1.06336500
47	-1.07080900	-3.35983400	-0.80490400



47	3.75459600	-1.87329200	0.25096300
47	1.80267900	2.83012000	1.06966800
47	-0.56570900	4.23307000	0.07907500
47	3.32593400	0.99344200	-0.72730300
7	5.47032300	0.22116700	-1.08608400
8	5.67464400	-0.99384500	-0.61848600
8	6.43254100	0.80774900	-1.62650300

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NO<sub>2</sub>\_Ag<sub>16</sub>  
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47	2.15511300	-3.54576600	-0.86906600
47	-1.00178900	0.13819300	2.60642200
47	0.64669500	-2.08568000	1.19257000
47	1.42063500	1.06550100	1.01265200
47	3.57661700	-1.14048000	0.32154000
47	-2.38325300	-2.17114700	1.30288200
47	-1.07068100	-0.06779100	-0.40688600
47	-2.62211900	2.02044500	-1.67345500
47	0.38606000	2.14338800	-1.72487200
47	-3.51126400	-1.29826800	-1.37524300
47	-0.85413600	-2.87570700	-1.27001800
47	-3.53664600	0.73885000	0.95252300
47	1.64658200	3.90693500	0.34204300
47	3.33851700	1.57539300	-1.11490900
47	-1.06762600	2.71715600	0.89793100
47	1.48727700	-0.73002400	-1.63899300
7	2.90607200	-0.76544300	3.43705100
8	1.74725800	-0.59294600	2.82085000
8	3.87629700	-1.03439500	2.66039600

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NO<sub>2</sub>\_Ag<sub>17</sub>  
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47	-0.03352400	-1.22636500	-2.79012600
47	1.33369000	2.27130200	1.29314000
47	-3.77436400	2.04981000	0.22613700
47	0.62816200	1.38393300	-1.81762400
47	-3.45349700	-0.93377300	0.53300300
47	3.53186900	0.19209900	1.34524900
47	2.56674700	-0.88931100	-1.28842400
47	-2.17153000	-2.80479300	-1.44601700
47	2.31167100	-2.51728600	1.29720900
47	0.82302100	-3.58741800	-1.16786900
47	-1.73459500	-1.53501300	2.79134300
47	3.46019500	1.97984900	-0.91971500
47	-1.42978000	1.21104900	1.77828700
47	-0.24674000	-1.13486800	0.16783700
47	1.03050200	-0.33837500	2.79361100
47	-2.19371600	0.47312800	-1.74717500
47	-1.13677600	3.30106800	-0.19263200
7	1.25684000	4.68948100	-1.88616500
8	1.71536900	3.46406400	-1.91584000
8	0.05579400	4.79930400	-1.46413300

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NO<sub>2</sub>\_Ag<sub>18</sub>  
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47	-3.00809800	-1.67919900	0.75567200
47	3.83629400	-1.03352600	-1.52973700
47	-0.71471700	0.84788400	-2.98450000
47	-2.19712600	2.31959100	1.37801900
47	-2.12615700	-1.69173200	-2.22149500
47	0.99741700	-1.61941700	-2.40028200
47	-0.17012800	2.76651500	-0.80298000
47	3.20620300	0.56299900	0.94910700
47	0.67311100	1.92068800	1.96885300
47	-0.54927800	-2.71333100	2.23392600

47	-1.44159400	-0.02818800	2.91014800
47	-0.46698100	-3.49284600	-0.62243000
47	1.56909100	-0.72445600	3.10012100
47	2.61060500	3.32200600	0.13282600
47	-3.28232000	0.75291100	-1.16597000
47	1.88858600	-2.07670100	0.47641900
47	2.06396500	1.22238700	-1.91756100
47	-0.63853600	-0.16238200	-0.00964100
7	-4.41551300	2.68262400	-0.66482900
8	-5.38799100	3.16702800	-1.27971800
8	-3.96917200	3.33810700	0.38979800

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NO<sub>2</sub>\_Ag<sub>19</sub>  
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47	1.38629900	2.40889300	2.55685800
47	-2.18088300	-1.13864600	-2.52656600
47	-2.86139800	-2.95825100	-0.08767300
47	-0.03469600	-3.28426800	-1.55452200
47	-0.15575900	3.67305400	0.04460000
47	-0.09289200	-3.31709500	1.53445500
47	-0.75942300	-0.91744200	-0.01186200
47	3.56217000	0.15545900	1.84709100
47	0.77134500	-0.57992000	2.50908300
47	-1.37870800	1.63802700	-1.79267800
47	-2.28842800	-1.22189200	2.41076700
47	3.65871400	0.21623700	-1.64216300
47	1.49434200	2.46719000	-2.43206500
47	0.88048500	-0.49998100	-2.43756800
47	-3.57499800	0.19337700	-0.04144600
47	2.21969200	-1.95881300	0.00780100
47	-3.27693300	3.10750700	-0.04849500
47	-1.43155000	1.58471600	1.73962400
47	1.47466400	1.14264200	0.05126600
7	5.70826900	-1.66393300	-0.12826500
8	4.59800800	-1.75290700	0.56748000
8	5.61150300	-0.96707700	-1.19846900

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NO<sub>2</sub>\_Ag<sub>1</sub>  
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7	2.03215200	0.00120800	-0.00009000
8	1.32345700	-1.08159200	0.00005300
8	1.32018600	1.08187900	0.00005300
47	-0.75264300	-0.00022900	-0.00000500

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NO<sub>2</sub>\_Ag<sub>20</sub>  
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47	-0.87336200	-1.72145600	-1.37070900
47	0.09215300	1.01944100	-0.31541800
47	1.01693400	3.61184600	0.63332700
47	0.88572000	1.16715700	2.53774400
47	2.98448800	1.28393100	0.30186300
47	3.99195000	-1.81479900	-0.54617400
47	-1.79812900	2.42646500	1.53737100
47	-1.58808900	0.93778000	4.15096100
47	1.57524100	2.48649600	-2.33295300
47	1.43624400	-1.34841200	0.95918800
47	1.82234600	-0.54191100	-2.15852700
47	1.60269500	-3.42267100	-1.11299900
47	-3.21079900	-1.15961700	-3.09124200
47	-3.47414800	-2.20345800	-0.15778200
47	-2.85778000	0.72689300	-0.83754300
47	-1.69884500	-0.58140900	1.61336800
47	-1.35885100	3.32035700	-1.40425900
47	0.20206600	-1.60174900	3.62028400
47	-0.85758000	0.75186300	-3.15519400

47	-0.78944900	-3.36480600	1.12129900
7	5.63383500	-0.29146800	-0.08012800
8	6.86552800	-0.50178300	-0.10582500
8	5.22588700	0.92166000	0.21938400

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NO<sub>2</sub>\_Ag<sub>21</sub>  
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47	4.97209700	-1.21295400	-0.51881800
47	1.57123900	1.15193500	2.65972900
47	3.62220100	-0.98646700	2.09507100
47	-2.11566000	-2.41290800	2.35128600
47	2.16440200	-2.12116000	-0.42970100
47	-2.55415200	-1.81777800	-2.35199700
47	-0.61331400	-2.88968800	-0.25731700
47	0.27136900	-1.12266500	-2.75133400
47	-0.08987800	0.07751900	0.02289500
47	0.79343100	-1.80866700	2.33099400
47	-1.39398900	0.43229600	2.73501000
47	2.88726500	0.92722100	-0.09829000
47	-0.96123900	3.89418300	-1.88446600
47	-2.16508400	2.43006200	0.52349800
47	1.04893800	1.77866600	-2.43648000
47	0.77362000	2.96352100	0.34315700
47	-1.91813300	1.08764100	-2.32303000
47	3.11722600	-0.35783200	-2.80267200
47	-0.58365400	3.26478100	2.96569400
47	-3.47373300	-3.51128300	-0.06410100
47	-3.05782800	-0.46742100	0.30288900
7	-5.09582500	1.59741300	-1.05483000
8	-3.93036700	2.19865800	-1.13619200
8	-5.09464000	0.52197700	-0.36143700

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NO<sub>2</sub>\_Ag<sub>22</sub>  
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47	-1.51753000	-2.77261100	0.61241200
47	0.70471500	-0.90042200	-0.31250800
47	-4.71868900	1.14636100	0.47564800
47	-1.48637600	-1.64747300	-2.36958000
47	-4.10926000	-1.55171100	-0.72762600
47	0.72204400	-3.59839400	-1.38990400
47	-3.28167800	1.12439000	-2.21463200
47	1.41723900	-1.14300400	-3.12010900
47	3.49495900	-1.83696500	-0.72355600
47	2.73001100	1.04522300	-1.25587400
47	2.77657200	-0.08832600	1.73368600
47	3.48606800	2.75151700	1.00818500
47	1.47838300	-3.04457900	1.49146500
47	5.29672900	0.40140800	0.17131800
47	0.58705600	1.88852100	1.07220800
47	-0.33579300	-0.59230700	2.52606300
47	-1.91140500	0.26452000	0.12675200
47	-3.38991800	-0.98278800	2.27038800
47	-0.16273600	1.32162100	-2.23621000
47	-2.18705900	2.02933100	2.38221900
47	1.29217300	3.71699700	-1.09029000
47	-1.68672600	3.21966900	-0.46472100
7	1.84751400	-1.64599500	4.58338400
8	2.41233700	-1.83790900	3.41101100
8	0.67826700	-1.13383400	4.53219000

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NO<sub>2</sub>\_Ag<sub>2</sub>  
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7	3.47206800	0.22417200	0.00036300
8	2.89442600	-0.93546200	0.00034300
8	2.63863900	1.21303700	0.00003900

47	-2.14898300	0.05079800	0.00010300
47	0.69006900	-0.13143200	-0.00022200

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NO<sub>2</sub>\_Ag<sub>3</sub>  
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7	3.29490600	0.00100000	0.00295800
8	2.60943900	-1.09544400	-0.00027100
8	2.60890900	1.09683100	0.00079700
47	0.35704200	1.39847700	-0.00064100
47	0.35851800	-1.39837600	-0.00049900
47	-2.09452000	-0.00048700	0.00061000

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NO<sub>2</sub>\_Ag<sub>4</sub>  
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47	2.71283900	0.51429000	0.00005200
47	0.73356600	-1.58393900	0.00000000
47	-0.02135000	1.21490500	-0.00011200
47	-2.03236500	-0.98365900	0.00000600
7	-3.19163000	2.03941200	0.00010800
8	-3.44832400	0.77659000	0.00002200
8	-1.94105500	2.36454400	0.00019900

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NO<sub>2</sub>\_Ag<sub>5</sub>  
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47	-0.00050100	-1.30792400	-0.00042100
47	-1.58902400	1.13881300	0.00598900
47	1.59035500	1.13889000	-0.00623500
47	-2.84086800	-1.34523800	-0.00415400
47	2.84025200	-1.34606200	0.00468500
7	-0.00030100	3.99248400	-0.00001700
8	1.09261500	3.31013900	-0.01484000
8	-1.09360800	3.31037400	0.01565200

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NO<sub>2</sub>\_Ag<sub>6</sub>  
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47	1.55977500	1.26979500	0.00144300
47	2.47046900	-1.36595200	-0.00102600
47	-0.00088500	-0.80021000	1.56408100
47	-2.47180200	-1.36376200	0.00114300
47	-1.55741500	1.27180500	-0.00217500
47	-0.00084800	-0.79977800	-1.56396700
7	0.00178300	4.12809600	0.00125500
8	1.09496800	3.44578100	0.00033900
8	-1.09238500	3.44723500	0.00151200

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NO<sub>2</sub>\_Ag<sub>7</sub>  
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47	0.54462900	2.45781500	-0.49444200
47	-2.20197700	1.48162300	0.34293800
47	-2.20380800	-1.48056300	0.34053800
47	-0.36190200	0.00100000	-1.61542300
47	0.05932000	-0.00182600	1.38656100
47	0.54371900	-2.45691900	-0.49720400
47	2.36818100	0.00068600	-0.67927900
7	2.12073200	-0.00335700	2.34593400
8	3.14242900	-0.00067300	1.51883800
8	2.35647800	-0.00706600	3.57429200

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NO<sub>2</sub>\_Ag<sub>8</sub>  
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47	0.47618700	0.64923400	-1.93507900
47	-0.97639400	1.38691600	0.91266500
47	-2.20568300	-0.41239600	-1.19538200
47	-1.51120300	-1.49398900	1.59844800
47	0.15959700	-2.00440100	-0.79424400

47	1.13735200	-0.38872600	1.85989700
47	1.85639700	2.00539400	0.37233100
47	2.80358500	-0.66979600	-0.64741700
7	-3.93264800	2.18454000	-0.36545200
8	-2.89322400	2.45835200	0.34736700
8	-3.88725800	1.08078700	-1.03351600

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NO<sub>2</sub>\_Ag<sub>9</sub>  
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47	2.22723500	1.26057900	-1.36695300
47	0.98434200	-1.44882600	-1.56672800
47	-0.99706100	1.00196200	-1.17151400
47	3.23182300	-0.64235300	0.42611500
47	1.11241300	1.03016700	1.63850600
47	-1.74418600	0.12191500	1.71399600
47	0.40747700	-1.79956600	1.36833500
47	-1.71612700	-1.78215000	-0.72916800
47	-3.71423500	0.60185400	-0.37509400
7	0.55490800	3.08587000	0.47579800
8	0.26231900	4.24011600	0.79958000
8	0.47601400	2.79120600	-0.84868500

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NO<sub>2</sub>  
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7	0.00000000	0.00000000	0.33130100
8	0.00000000	1.13585900	-0.14494400
8	0.00000000	-1.13585900	-0.14494400

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NO\_Ag<sub>10</sub>  
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47	0.41797100	1.65468800	1.14152000
47	2.45652700	-0.96347800	0.84022100
47	-2.06248400	0.01125100	1.04417100
47	0.14459200	-0.78905100	2.85521400
47	-0.10930900	-2.12753100	0.20550300
47	-2.64684600	-1.83248900	-1.16224600
47	-2.00289800	2.73952400	-0.08372000
47	-0.75354200	0.44397000	-1.60972800
47	1.90118100	1.62278900	-1.55205800
47	1.64343700	-1.26603200	-1.97266300
7	2.74945400	2.08209800	0.69187800
8	3.53602100	1.15302800	1.12060000

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NO\_Ag<sub>11</sub>  
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47	0.64916400	-2.71530400	-0.48035900
47	-1.26880000	-1.25892100	1.37507300
47	-3.82434800	-1.52284100	-0.10751300
47	-1.29247500	-0.65091100	-1.56037900
47	1.53755800	-0.16315000	-1.66564500
47	-0.14762100	2.22408500	-1.25267300
47	-2.96110800	1.13650700	0.30499300
47	-0.14088200	1.45247000	1.76833900
47	1.65616500	-0.87359700	1.51524600
47	2.45401600	1.78003300	0.29026300
47	4.09117300	-0.59456800	-0.07762800
7	-2.11584000	3.10554800	-0.43333400
8	-2.57158400	4.25155000	-0.26542600

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NO\_Ag<sub>12</sub>  
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47	1.05588200	0.05563100	-1.17679800
47	-2.31139400	0.06595100	-1.50623500
47	-0.79945400	-2.52690300	-0.20380300
47	1.24048800	-1.40786500	1.69600100

47	1.30559100	1.47945400	1.68527100
47	-1.29477000	0.06264200	1.36687200
47	-3.39752900	2.00237600	0.24229600
47	-0.60288800	2.49321400	-0.42606300
47	-3.50842800	-1.70438000	0.51953900
47	2.46658500	2.55559400	-0.84709200
47	3.62898500	-0.02719700	0.22189000
47	2.37614500	-2.58164500	-0.71210500
7	-0.46160000	-2.16729200	-2.67345700
8	-0.53147800	-0.84649300	-2.71188900

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NO\_Ag13  
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47	1.13832700	-0.03584600	-1.21160100
47	3.28509300	1.86281900	-0.71542300
47	1.85326600	-2.94096600	-1.09214300
47	1.70561400	1.07868500	1.82007200
47	3.57446800	-0.90178500	0.19855100
47	0.14553400	2.67431500	-0.39087600
47	-1.17126500	0.40855200	1.09629600
47	-1.09090900	-2.02533400	-1.12659600
47	0.78829700	-1.76040700	1.39569300
47	-3.75661100	-0.49537000	-0.22070900
47	-1.56546600	0.80662800	-1.92845300
47	-2.28022700	-2.25188600	1.58648300
47	-3.09232300	2.39671400	0.03989500
7	1.76211200	3.37559900	2.22221900
8	1.19708300	4.00165100	1.27982000

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NO\_Ag14  
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47	1.00276000	-0.67519700	-1.39956500
47	0.36960600	2.13620900	-1.67035200
47	3.16141000	1.77359900	-0.56547700
47	-1.79608500	0.22064400	-1.58740700
47	-1.56163100	-0.37530800	1.32349700
47	-3.93930800	1.18620900	0.29450100
47	-3.73008500	-1.73051400	-0.25488800
47	1.30401900	3.90012900	0.55348200
47	1.04210000	0.99573200	1.28675700
47	3.48135700	-1.04529500	0.09357500
47	-1.44103800	2.64471200	0.65128800
47	0.91662500	-1.93686300	1.43087900
47	-1.04313900	-2.78498600	-0.67058900
47	1.89983100	-3.50306600	-0.84699400
7	1.29846600	-2.48127100	3.68369600
8	0.82361800	-2.56415900	4.77437400

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NO\_Ag15  
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47	2.03673800	-3.67944400	0.01577800
47	-1.74044100	0.53628400	-1.42131600
47	0.22345900	-1.72927800	-1.40230000
47	-2.75779900	-2.25732200	-0.83571400
47	-0.70561300	-3.38661900	0.98119200
47	1.21071900	1.03962700	-1.27438600
47	1.21456600	-0.99596500	1.27104400
47	0.17979200	1.76043400	1.37951400
47	-1.72272300	-0.54568000	1.40098900
47	3.27936300	1.30346500	0.99485000
47	3.24310300	-1.23047600	-1.00480700
47	1.96162100	3.71706700	-0.03722900
47	-2.84280300	2.21755200	0.78327500
47	-4.49135200	-0.09615500	0.10589100
47	-0.79930300	3.36864600	-1.01606200

7	5.37034100	0.39760200	0.67534900
8	5.35115600	-0.47794400	-0.24265200

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NO\_Ag<sub>16</sub>  
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47	-0.19845000	3.50566700	0.55478700
47	1.29722000	-1.98235400	2.22246500
47	0.50991300	0.86781400	1.77492100
47	-1.84828600	-1.03990000	1.65050700
47	-2.31432600	1.81773600	1.81785100
47	3.32898300	-0.09326200	1.52118800
47	0.61468400	1.54047800	-1.58952600
47	1.20935300	-1.20338200	-2.55838400
47	-1.57069800	-0.40620800	-1.79979200
47	3.48204000	0.43187300	-1.54547200
47	2.64708400	2.59150400	0.32940400
47	2.80909200	-2.26355500	-0.36304900
47	-3.22579400	-2.52153500	-0.70199500
47	-3.93493000	0.29874800	-0.10842700
47	-0.22808400	-2.78155100	-0.50149500
47	-2.26933700	2.41883000	-1.40259700
7	-0.69763200	-3.16570800	1.88322900
8	-1.20180500	-4.16780600	2.46240700

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NO\_Ag<sub>17</sub>  
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47	2.75738000	0.75847800	-1.98764400
47	-0.54059300	-1.87743800	2.73658600
47	-0.56392600	3.18285300	2.17247600
47	3.56919100	0.54948900	0.88159500
47	-1.26727700	1.62887600	-0.15502900
47	0.39105200	-3.12535000	0.00477100
47	2.89341300	-2.00053600	-0.97740400
47	-0.03322900	1.95781400	-2.82087800
47	-1.82486300	-3.04472900	-1.99189700
47	0.28080900	-0.82240600	-1.88860100
47	-4.11552600	0.84453700	0.13728000
47	2.36686200	-2.03284200	1.92300800
47	-2.21623900	0.58387500	2.46138800
47	-2.46233300	0.15170600	-2.31964200
47	-2.28127500	-1.44976900	0.33395100
47	1.65293900	2.74927500	0.13448600
47	0.90297300	0.60751100	2.05265400
7	1.29888500	3.61817900	-1.95108900
8	1.74599200	4.69870100	-2.38825100

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NO\_Ag<sub>18</sub>  
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47	3.52384200	0.70928800	0.77909100
47	-2.24705500	-3.23657000	-0.72434400
47	-0.82973100	-0.06620300	2.97575300
47	0.33216800	3.98425000	0.14850700
47	1.97776900	-0.96466100	2.71301800
47	-0.38699000	-2.67140200	1.53999300
47	-1.66377000	2.08574000	1.17475800
47	-1.99184800	-0.66384900	-2.13340400
47	-0.97150200	2.24026700	-1.85404200
47	2.97865900	-0.80140700	-1.72388200
47	2.05283500	2.12237500	-1.42406200
47	2.36622000	-2.78550300	0.39282400
47	0.58449400	0.16258900	-3.20669200
47	-3.67624900	1.43530700	-0.90603400
47	1.22132700	2.00927200	2.21618000
47	0.42746800	-2.53694600	-1.87845800
47	-2.72618900	-0.78504200	0.85737000

47	0.59939300	-0.14241400	0.09023100
7	-4.59827000	-0.75858000	2.72414900
8	-5.20521200	0.10510000	3.27513100

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NO\_Ag19  
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47	2.68904000	0.96417200	-2.62243200
47	-1.36879100	-2.05383700	2.46956300
47	-3.34447400	-2.25910100	0.13152600
47	-3.16773400	0.46869200	1.79252600
47	3.70828800	-0.62698500	-0.11711300
47	-3.52599200	0.42892000	-1.36164700
47	-1.03949400	-0.49296500	0.05634700
47	0.70525800	3.66477600	-1.56326100
47	-0.48238900	1.03093500	-2.39799900
47	1.49065800	-1.50722500	1.64265400
47	-1.66328600	-1.87426600	-2.37302700
47	0.97721900	3.60378600	1.64792200
47	2.85554300	1.06984300	2.36255000
47	-0.26939300	1.02097800	2.49364200
47	-0.27716700	-3.41794700	-0.04582500
47	-1.53410900	2.70488700	0.18073000
47	2.82377700	-3.47068000	-0.09534300
47	1.33219900	-1.55408500	-1.83732000
47	1.38927200	1.29752800	-0.07370800
7	-3.61883900	2.66231900	-0.81257200
8	-4.46175900	3.56059500	-0.99147400

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NO\_Ag1  
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7	0.49671900	-1.54748400	0.00000000
8	-0.43462900	-2.34092800	0.00000000
47	0.00000000	0.62893200	0.00000000

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NO\_Ag20  
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47	1.99231600	1.44327900	-1.46229700
47	-0.06010400	0.00526000	0.53742100
47	-1.27309200	-1.19167600	3.28110900
47	-2.17774900	-2.10219400	0.55095000
47	0.72509800	-2.72047000	1.55309800
47	2.77495300	-3.54403900	-0.50591400
47	-2.86346500	0.73280200	1.52649500
47	-4.62506200	-0.70463000	-0.48236200
47	1.62654900	-0.35513400	3.25069000
47	0.09958400	-2.59367000	-1.37990300
47	2.83832600	-0.72672800	0.49757200
47	2.57629700	-1.27521200	-2.48107800
47	1.53098600	4.25061400	-0.63802500
47	-0.40668200	2.90271100	-2.53581000
47	-0.87811300	2.87253000	0.44464700
47	-2.43404300	1.04630600	-1.41352900
47	-0.54201700	1.73194900	3.22328700
47	-2.54660500	-1.79143100	-2.41760100
47	1.92830700	2.10195400	1.46526200
47	-0.13594300	-0.06778000	-2.99322000
7	5.34671300	-0.04638200	0.37758200
8	6.19308000	-0.04423800	-0.45253300

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NO\_Ag21  
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47	4.30513500	-2.33483700	-0.84763100
47	2.04688300	1.79213600	1.84639600
47	3.73138100	-1.08097400	1.78490000
47	-2.12988000	-1.05883400	3.20573100



47	1.54368400	-2.42979600	0.06526800
47	-3.56750000	-1.90510000	-1.56495100
47	-1.26458900	-2.58546100	0.71548400
47	-0.65625700	-1.95060500	-2.16414700
47	-0.05077300	0.17870200	0.05019300
47	0.78870800	-0.95229700	2.74420100
47	-0.92582400	1.58852300	2.59765700
47	2.80236200	0.28825600	-0.80736600
47	-0.95915800	3.21945400	-2.99088200
47	-1.77940000	2.73508800	-0.13469800
47	0.65930400	0.70767800	-3.02580900
47	1.15280500	2.80069400	-0.87293100
47	-2.32106800	0.64128100	-2.33817500
47	2.18535600	-1.82891400	-2.90857900
47	0.18409600	4.16889700	1.59713000
47	-4.08710600	-2.48668900	1.40438300
47	-3.01593600	0.17032500	0.60305000
7	4.58786300	0.42409700	3.29134700
8	3.96257100	1.52344900	3.23462500

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NO\_Ag<sub>22</sub>  
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47	-1.69695800	2.61337700	-0.91586800
47	0.66690700	0.99287000	0.11501300
47	-4.45178600	-1.68906800	-0.26536000
47	-1.44805800	1.59707600	2.16290000
47	-4.27405500	1.11671000	0.60188900
47	0.48791400	3.73265100	1.03596200
47	-2.99514000	-1.14207300	2.39302000
47	1.54103300	1.46687700	2.85821300
47	3.38673200	2.16611400	0.31569000
47	2.92273700	-0.70435400	1.19679000
47	2.71885800	0.13665000	-1.94058900
47	3.70580600	-2.55719400	-0.95993600
47	1.28289600	2.91989400	-1.94655300
47	5.35680800	0.06614200	-0.41202200
47	0.80624500	-1.93240100	-0.98846900
47	-0.28062600	0.36170100	-2.66227800
47	-1.81629800	-0.43733000	-0.13243800
47	-3.30932200	0.42107000	-2.44275700
47	0.09759800	-1.15596900	2.26741200
47	-1.86432100	-2.38067600	-2.29304300
47	1.76858800	-3.48217900	1.33159400
47	-1.32198100	-3.28599000	0.65955500
7	-4.50865300	3.37992100	0.41910000
8	-3.59594800	3.95217600	-0.24170600

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NO\_Ag<sub>2</sub>  
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7	3.05632100	0.12380800	0.00129100
8	3.69517100	1.13269300	-0.00056300
47	-1.84232600	0.23404400	0.00006200
47	0.75816400	-0.44528200	-0.00015800

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NO\_Ag<sub>3</sub>  
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47	-1.91369900	-0.00018500	0.00195200
47	0.49510300	1.51989600	-0.00193500
47	0.49514000	-1.51955200	-0.00193700
7	2.23610600	-0.00045700	0.00549300
8	3.46871000	-0.00053500	0.00647500

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NO\_Ag<sub>4</sub>  
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47	2.29746500	-0.76991100	-0.06571300
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47	0.01423900	1.17903800	0.02766500
47	-0.45444100	-1.56396600	0.07517700
47	-2.65762000	0.36714300	-0.04595300
7	2.05486200	2.13861200	-0.29245900
8	2.90409300	2.75643200	0.30774400

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NO\_Ag<sub>5</sub>  
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47	1.50550300	1.39588800	-0.39349000
47	-2.66483100	-1.13756000	-0.35641300
47	-0.00017600	-1.03195300	0.82471700
47	-1.50670700	1.39623800	-0.39101500
47	2.66603200	-1.13640900	-0.35513700
7	0.00019500	1.23554000	1.56322400
8	0.00087200	1.93744800	2.57629400

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NO\_Ag<sub>6</sub>  
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47	-0.80534400	-1.50859000	-0.16897800
47	-3.20447900	-0.00398700	-0.36280200
47	-0.80933000	1.50659100	-0.16649700
47	1.68376300	2.83552200	-0.09389400
47	1.76948700	0.00242100	-0.06101000
47	1.69143100	-2.83085100	-0.09334700
7	-0.74374700	-0.00279300	2.39489000
8	-1.26169700	-0.00405100	3.46531700

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NO\_Ag<sub>7</sub>  
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47	2.52961100	0.00126500	-0.36070400
47	0.64172900	-2.45112000	-0.35901400
47	-2.20122000	-1.46083800	0.15702500
47	-0.08618800	-0.00091700	1.53986900
47	-0.10643100	0.00107500	-1.58076500
47	-2.20280500	1.45807400	0.15834300
47	0.63888700	2.45288200	-0.35743200
7	2.14111400	-0.00061500	1.93603300
8	2.74672900	-0.00192700	3.02170400

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NO\_Ag<sub>8</sub>  
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47	-0.38099100	0.64793200	-1.87155700
47	-0.57598700	-2.08642100	-0.56129000
47	1.99746900	-0.90814300	-1.47842700
47	1.56706000	-1.63954900	1.47897600
47	1.38942100	1.19579500	0.56904500
47	-0.92395300	-0.28149600	1.88525400
47	-2.81701700	-0.30081600	-0.43198500
47	-1.28926700	2.26961100	0.43804200
7	3.13511400	2.95915400	0.29485700
8	3.32721200	3.89137500	-0.42283400

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NO\_Ag<sub>9</sub>  
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47	1.44134400	-2.63332400	-1.25346300
47	0.56097800	-1.83822000	1.50280000
47	-0.19210700	-0.29124200	-1.02765900
47	2.67148300	-0.28465100	-0.11796100
47	1.12823800	2.59453200	-0.46934600
47	-1.69522600	2.04219900	-0.37167600
47	0.08410100	1.03145600	1.84228600
47	-2.16160800	-0.86261400	1.35771200
47	-3.08053900	-0.44784500	-1.35567000
7	3.29904100	1.87296000	-0.34403400
8	4.41794000	2.41319800	-0.32773000

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NO

7	0.00000000	0.00000000	-0.63193500
8	0.00000000	0.00000000	0.55294300

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SO<sub>2</sub>\_Ag<sub>10</sub>

47	0.56502100	-1.64375400	0.48588800
47	3.06691300	0.21226200	0.49264400
47	-1.50285200	-1.05055100	-1.54139700
47	2.63524800	-1.73103600	-1.60465400
47	1.02056800	0.64829200	-1.77494000
47	-1.48308900	2.14669300	-1.36214600
47	-2.24012600	-2.19679600	1.08531600
47	-1.44452600	0.69850300	1.26413100
47	1.13774800	0.34299100	2.67011400
47	0.84414600	2.42513900	0.48979100
16	-4.37695800	0.29193700	-0.35840600
8	-3.07036800	0.57431900	-1.49138100
8	-3.44513600	-0.28718000	1.00530000

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SO<sub>2</sub>\_Ag<sub>11</sub>

47	1.52032200	-2.41989900	-0.19293200
47	-0.91149100	-1.50001400	1.40678200
47	-3.44887100	-2.29699400	-0.21279100
47	-0.97993600	-1.09576300	-1.51804700
47	1.65685900	-0.03307700	-1.89104800
47	-0.46584700	1.88027900	-1.50362400
47	-3.03181100	0.40039700	0.21947200
47	-0.44876800	1.53451600	1.64084100
47	1.70248700	-0.36666700	1.88554600
47	2.16518000	1.98190800	0.18713700
47	3.96567900	-0.40835600	-0.05542300
16	-2.73412000	3.85375800	0.19217400
8	-2.07637800	3.50106800	-1.26428200
8	-2.58273100	2.44298300	1.08019300

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SO<sub>2</sub>\_Ag<sub>12</sub>

47	-0.79540800	-1.70732900	1.23217400
47	1.84361700	-1.56029000	-0.28629300
47	-0.91410400	-1.21779500	-1.59719000
47	-2.17108500	1.38024100	-2.26578500
47	-1.35220900	2.42828700	0.37492800
47	0.71403800	1.20408600	-1.59387100
47	3.77328200	0.71804500	-0.23974700
47	0.97074700	0.63920400	1.52411300
47	4.71297800	-1.85872800	0.13101400
47	-1.77977500	0.62602400	2.75497500
47	-3.13602600	0.02097300	0.19461200
47	-3.07764500	-2.80649000	-0.36753200
16	1.97358100	3.66723900	0.24934700
8	2.45023000	2.36647300	-0.82352800
8	0.72070200	2.83495300	1.13911500

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SO<sub>2</sub>\_Ag<sub>13</sub>

47	1.30489300	-0.43333800	1.13047900
47	2.97612400	-2.65201200	0.17551900
47	2.70452800	2.12563500	1.66069000
47	1.90867100	-0.84847300	-1.95206600
47	4.10460800	0.09108700	0.22712000
47	-0.19127000	-2.50520100	-0.50160500

47	-0.89999200	0.13655700	-1.46278900
47	-0.56063800	1.82100300	1.16063800
47	1.52657800	1.86508300	-1.08821000
47	-3.45276300	1.05118500	-0.08421800
47	-1.54349100	-0.93867100	1.68325500
47	-1.78511900	2.94971400	-1.30634700
47	-3.02627900	-1.87096800	-0.93882100
16	-4.93414100	-1.31586200	2.11195800
8	-4.68481600	-0.75559300	0.56100200
8	-3.45877700	-1.26335000	2.83116700

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SO<sub>2</sub>\_Ag<sub>14</sub>  
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47	-0.78201900	0.51740000	-0.65350300
47	-0.60310700	-2.08640800	-1.85110700
47	-3.39560100	-0.21925400	-1.86661600
47	1.82272400	-0.34252800	-1.63345500
47	1.91058300	0.38244600	1.29050300
47	4.06280100	-1.37029100	0.02921800
47	3.95370700	1.60991000	-0.42342300
47	-2.91309800	-1.86567600	0.40454700
47	-0.53734300	-0.86371800	2.25868100
47	-3.28368000	1.18013400	0.70280100
47	1.44970900	-2.59531000	0.35954500
47	-0.46801000	2.01325300	1.87905600
47	1.25746600	2.66345800	-0.69572900
47	-1.70110700	3.45631500	-0.39344900
16	-0.73939600	-4.04504400	0.98980300
8	-1.54586100	-3.63019700	-0.50081800
8	-1.51686900	-2.84812500	2.00468200

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SO<sub>2</sub>\_Ag<sub>15</sub>  
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47	-0.44990800	3.91887600	-0.13493200
47	0.20975600	-1.54268000	1.43167900
47	-0.14088800	1.40275400	1.54798800
47	-2.58283600	-0.35429700	1.29447100
47	-2.36438900	1.63562300	-1.08920000
47	2.59600400	0.15541000	1.22573900
47	0.70851300	1.35070900	-1.36943700
47	1.96290000	-1.30675700	-1.33179300
47	-1.02347300	-0.98964200	-1.31578600
47	3.72056800	1.12230800	-1.33424200
47	2.26053800	3.14186200	0.36246900
47	2.90859100	-2.85391600	1.04546800
47	-2.27576500	-3.11035400	0.32140400
47	-4.01983800	-0.79411600	-1.22031900
47	0.48876900	-3.77516700	-0.50145400
16	-3.24483000	3.20558700	1.86620000
8	-2.46297000	1.78963500	2.23441600
8	-2.78879400	3.54559300	0.30736100

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SO<sub>2</sub>\_Ag<sub>16</sub>  
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47	-2.55521500	3.56111200	-0.24236300
47	0.66114500	-0.20379500	2.75065100
47	-1.00090500	1.77959300	1.44090900
47	-1.57909100	-1.11295100	1.13939000
47	-3.80630100	0.95395600	0.78586900
47	2.45369100	2.05756400	1.14316400
47	0.82751200	0.16606700	-0.37164000
47	2.24436800	-1.35311800	-2.38935500
47	-0.71154500	-1.90555700	-1.72656800
47	2.97211600	1.59974800	-1.80248000
47	0.41676100	3.12044900	-0.83251400

47	3.85961500	-0.63594700	-0.07130300
47	-1.62916900	-3.93314200	0.23118700
47	-3.60400600	-1.58654500	-0.83679000
47	1.07402000	-2.76263700	0.63975200
47	-1.84321400	0.85543700	-1.49309500
16	3.18306900	-0.96769500	2.96773800
8	2.97148600	-2.02907700	1.59433900
8	3.70615900	0.43809700	2.076901004

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SO<sub>2</sub>\_Ag<sub>17</sub>  
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47	1.52074600	3.42280100	-0.85613600
47	0.38339600	-3.55382400	-1.10850100
47	2.97307000	-1.03595500	2.61480700
47	2.89149600	1.01013900	-1.87977800
47	0.25371200	0.14016400	2.35483400
47	-1.33217000	-1.67766700	-2.84061700
47	-0.02226200	0.84679100	-1.81008800
47	0.03910000	3.03070300	1.73470600
47	-2.89870000	0.65907500	-1.71898000
47	-1.54346000	3.21215800	-0.84209200
47	-2.13971000	-1.47607400	2.81167600
47	1.78728400	-1.54347300	-2.89480300
47	0.39530000	-2.85304500	1.83428500
47	-2.28109600	1.32528900	1.34782500
47	-1.48730800	-1.44076500	-0.00234900
47	2.56822200	1.57803500	1.16843800
47	2.15973300	-1.36564900	-0.08870200
16	-5.23583800	-0.59647800	0.43119500
8	-4.99120400	0.12104100	-1.01953700
8	-3.73281600	-0.56546800	1.18807100

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SO<sub>2</sub>\_Ag<sub>18</sub>  
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47	-0.56501100	0.00195800	2.92326200
47	-3.13467900	0.00742100	-2.20084400
47	-0.14883800	3.72526700	-0.16315800
47	3.30896500	-0.00915200	1.42131500
47	-1.77961600	2.56380900	2.05775000
47	-2.84779500	2.63791700	-0.82407200
47	2.38718400	2.52014000	-0.70237500
47	-0.36492900	-1.53511600	-2.18741700
47	2.37378000	-2.53271000	-0.70296900
47	-1.79293200	-2.55416800	2.05836800
47	1.26119500	-2.22892400	2.05781500
47	-2.48955300	0.00647600	0.65630900
47	-0.16814000	-3.72546100	-0.16227600
47	2.21852400	-0.00553500	-2.57049800
47	1.27263900	2.22346900	2.05864000
47	-2.86167700	-2.62348400	-0.82321600
47	-0.35721400	1.53681800	-2.18894600
47	0.67916000	-0.00071300	0.12033000
16	4.85719600	-0.01287300	-0.83953600
8	3.98478400	1.29036700	-1.59270500
8	3.97833300	-1.31170400	-1.59281800

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SO<sub>2</sub>\_Ag<sub>19</sub>  
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47	1.66919700	1.50029800	3.18845300
47	-1.87292300	-0.12146200	-2.94223900
47	-3.92839700	-1.06956000	-0.79322500
47	-1.55430800	-2.99591800	-1.46477300
47	1.89032800	3.12623700	0.19315200
47	-2.22325000	-2.66804000	1.58336600
47	-1.14988700	-0.47084400	-0.11467700

47	2.57376100	-1.56698200	2.67021000
47	-0.34201100	-0.74783200	2.88402900
47	0.18925600	1.78115300	-1.86605500
47	-3.16270800	0.30379100	1.78091000
47	3.45394900	-1.84995100	-0.25082900
47	3.12203600	1.12095400	-1.73291000
47	0.91121400	-1.20632200	-2.09160300
47	-2.72427800	1.94329000	-0.81237300
47	0.71426200	-2.72053100	0.61960100
47	-0.85410600	4.26857500	-0.61523100
47	-0.71614900	2.17027100	1.49868900
47	1.62026400	0.25297300	0.59825400
16	3.83437900	-1.68947400	-3.77846100
8	4.13508600	-0.92524300	-2.31572300
8	2.20069700	-1.86514000	-3.83225400

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SO<sub>2</sub>\_Ag<sub>1</sub>  
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16	-1.99505300	-0.00074000	-0.00013800
8	-0.93097300	1.27729600	0.00021400
8	-0.92793300	-1.27701300	0.00021400
47	0.99557600	0.00020400	-0.00002600

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SO<sub>2</sub>\_Ag<sub>20</sub>  
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47	-2.31373000	1.27073200	-1.45290100
47	0.38282600	0.17800600	-0.40883800
47	1.70385700	-0.64976100	3.66450700
47	2.94788100	-0.59408700	0.90339900
47	1.78095500	2.04018500	1.95931700
47	1.52903500	4.45036300	0.01586600
47	0.65431800	-2.46221200	1.57387800
47	2.64547300	-3.27922800	-0.31638200
47	-0.69483400	0.52387800	2.49856900
47	2.87016400	1.92514200	-0.87792400
47	-0.85460800	2.91565000	0.70771100
47	0.18399300	2.76525800	-2.11166300
47	-4.76448500	-0.25029600	-0.56750200
47	-2.73998000	-1.58109500	-2.21508500
47	-2.13937200	-1.45928500	0.70453000
47	-0.18187100	-2.73733200	-1.30344200
47	-1.29775500	-2.00624400	3.68683000
47	2.78630200	-0.63283700	-2.23052600
47	-3.31550000	1.33099700	1.36100400
47	-0.33533100	0.04924100	-3.29941500
16	1.36295500	-3.09061400	-3.52375300
8	1.23842200	-1.38494500	-3.87538100
8	2.80756300	-2.99164000	-2.54220900

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SO<sub>2</sub>\_Ag<sub>21</sub>  
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47	-4.66921000	-1.85351400	-1.08634500
47	-0.90962400	1.58780800	-2.54878200
47	-2.64370500	-0.80676600	-3.08864100
47	3.03477400	-1.52902100	-1.97604100
47	-1.80245400	-2.37668000	-0.58784800
47	2.02531200	-2.13178200	2.73388100
47	1.04446500	-2.74955400	-0.06123700
47	-0.90445600	-1.87444200	2.24492000
47	-0.02002000	0.10775600	0.00019300
47	0.29431600	-1.17997800	-2.75573800
47	2.09323600	1.36875800	-2.02390800
47	-3.04213800	0.57068400	-0.46945000
47	-0.42984700	3.36184800	2.96874300
47	1.48038100	2.64126400	0.75735800

47	-2.10162300	0.97220500	2.37862400
47	-1.42593700	2.94447500	0.16113700
47	0.86031500	0.63147400	2.94368600
47	-3.82804500	-1.35949800	1.70596400
47	0.63118000	4.00022600	-1.76671600
47	3.95638500	-2.79234100	0.59082100
47	2.88254900	0.03117700	0.77054100
16	5.59893400	0.73963700	-1.31263800
8	4.42372200	1.63210200	-2.02246300
8	4.78901000	-0.55045500	-0.58784700

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SO<sub>2</sub>\_Ag<sub>22</sub>  
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47	1.35186000	2.54198100	1.49160700
47	-0.80491600	1.00300600	0.04490300
47	4.43239700	-1.66389400	0.76465100
47	1.43825800	2.20267400	-1.58834800
47	4.52590700	1.09380400	-0.22925400
47	-0.79871800	3.87997700	-0.40831600
47	3.16199400	-1.07272000	-2.23470900
47	-1.47948900	1.81463200	-2.59150400
47	-3.62884700	2.04565600	-0.33552700
47	-2.91210300	-0.66594200	-1.50965000
47	-3.02041800	-0.17111300	1.73063900
47	-3.77648300	-2.74063500	0.46306200
47	-1.81144200	2.59200200	2.22114100
47	-5.49950900	-0.26156900	-0.07855000
47	-0.89535700	-2.12440200	0.90196500
47	0.06422400	0.06594500	2.73396600
47	1.81097000	-0.33499800	0.24346600
47	3.29260200	0.41950500	2.56627900
47	0.06711500	-0.84968600	-2.16885000
47	1.71183700	-2.47249500	2.30261000
47	-1.57377600	-3.34680700	-1.71221300
47	1.47744600	-3.09923300	-0.77713100
16	4.22290000	1.87987200	-3.24439700
8	3.60593500	2.58301600	-1.74010600
8	4.78863800	0.38007200	-2.52374000

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SO<sub>2</sub>\_Ag<sub>2</sub>  
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16	-0.73698000	1.63326300	-0.44563900
8	0.92688300	1.78038000	-0.14518400
8	-1.53429300	2.37086500	0.74400300
47	1.60682500	-0.29147100	0.05866800
47	-1.25254900	-0.97112900	-0.00888800

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SO<sub>2</sub>\_Ag<sub>3</sub>  
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16	-3.34245300	-0.00004200	-0.00014200
8	-2.37678100	-1.33562400	0.00079000
8	-2.37676300	1.33563200	-0.00033600
47	2.27346900	-0.00006600	0.00000700
47	-0.16320900	1.41053000	0.00007300
47	-0.16329000	-1.41045100	-0.00010900

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SO<sub>2</sub>\_Ag<sub>4</sub>  
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47	0.11934300	-1.51064100	-0.86962800
47	2.22158400	-0.00057700	0.37609000
47	-0.81870400	-0.00003900	1.60186100
47	0.12003100	1.51128900	-0.86903800
16	-2.91380100	-0.00002600	-0.66425700
8	-1.91046200	-1.31049200	-0.03851900
8	-1.91017600	1.31036000	-0.03877100

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SO<sub>2</sub>\_Ag<sub>5</sub>

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47	0.63551000	-1.08935000	-0.00135900
47	-1.20430700	1.13178700	-0.00178400
47	1.87187000	1.47393200	0.00057600
47	-2.19424200	-1.51336900	0.00039600
47	3.77062800	-0.52326000	0.00095600
16	-4.68099100	0.93426300	0.00149900
8	-3.30428200	1.84339300	0.00182200
8	-4.25055600	-0.65539500	0.00232800

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SO<sub>2</sub>\_Ag<sub>6</sub>

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47	0.51398800	-1.46890800	-0.00154800
47	3.27075700	-1.00286500	-0.00005000
47	1.58600500	1.30386500	-0.00058600
47	-1.29736400	0.48324600	-1.48449300
47	-1.29492900	0.47990200	1.48636800
47	-2.46364600	-1.71047400	-0.00042700
16	-0.80016400	3.30375700	0.00149700
8	-0.12478200	2.32322700	-1.30724500
8	-0.12440200	2.32125900	1.30858200

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SO<sub>2</sub>\_Ag<sub>7</sub>

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47	1.90805200	-1.69630500	0.36453600
47	1.19306400	2.29807000	0.25376500
47	-1.65095700	1.85700200	0.38531200
47	-0.06762600	-0.03216300	-1.28441200
47	0.30607200	0.12699500	1.93480000
47	-2.86594000	-0.47402200	-1.02018600
47	-0.91402300	-2.20258000	0.50635600
16	3.43235400	0.36246000	-1.96002700
8	1.93679000	1.04040400	-1.65529700
8	3.48523700	-1.04268500	-1.12314500

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SO<sub>2</sub>\_Ag<sub>8</sub>

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47	2.21695500	0.87681200	-0.95114800
47	0.01724900	-1.22431000	-0.96408600
47	2.78464800	-1.89133200	-0.12361400
47	-2.73843200	-1.90969300	-0.25734000
47	1.36599000	-0.19255400	1.76310400
47	-1.52993300	-0.02343500	1.79322600
47	-2.20253800	0.82147100	-0.96629000
47	0.00659200	2.27221300	1.07850100
16	-0.31535700	2.11629200	-2.30490300
8	0.38469700	0.52379900	-2.43548600
8	0.71289200	2.70972900	-1.01728400

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SO<sub>2</sub>\_Ag<sub>9</sub>

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47	3.42385400	-0.00010000	0.00115200
47	1.64412500	1.52898500	1.84049000
47	0.91426900	-1.24524100	1.02553700
47	0.91545900	1.24509300	-1.02581300
47	1.64588300	-1.52904100	-1.84018000
47	-1.19561100	-0.82797500	-1.35850900
47	-1.75791800	2.13692000	-1.28094900
47	-1.19670500	0.82781600	1.35873600
47	-1.75970400	-2.13672400	1.28037400
16	-4.37763200	0.00043700	-0.00131900
8	-3.35856400	1.26859400	0.34622900
8	-3.35887100	-1.26790600	-0.34851700

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SO <sub>2</sub>			
16	0.00000000	0.00000000	0.43436600
8	0.00000000	1.30436500	-0.43436600
8	0.00000000	-1.30436500	-0.43436600

**Table S2**

The XYZ coordinates of optimized structures of isolated Au<sub>n</sub> (n = 1-20) clusters, isolated gases including CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, and SO<sub>2</sub> as well as the gas/cluster complexes at M06-2X/SDD level of theory

Au <sub>10</sub>	X	Y	Z
79	-4.26731400	-0.00000100	0.00010300
79	1.45036900	0.00000000	-0.00008300
79	2.84030500	2.43905600	-0.00003200
79	-1.45037000	-0.00000000	-0.00007700
79	0.00000100	-2.43502400	-0.00012700
79	4.26731300	0.00000100	0.00011400
79	2.84030700	-2.43905500	0.00007700
79	-2.84030400	-2.43905600	0.00002100
79	-0.00000100	2.43502500	-0.00003400
79	-2.84030700	2.43905500	0.00003700
Au <sub>11</sub>			
79	-3.70429600	-1.79833300	0.00013000
79	1.16946700	-2.66113300	0.00011600
79	-1.49089400	-3.67563300	-0.00001000
79	2.12992700	2.87432500	0.00011400
79	-2.83951400	3.61487800	0.00010500
79	4.28992400	1.06694000	0.00016500
79	-0.56506300	2.02243700	-0.00033500
79	1.57051400	0.14644900	-0.00002800
79	-3.30883400	0.94231400	-0.00002900
79	3.80479000	-1.66792400	-0.00016500
79	-1.05602200	-0.86432000	-0.00006500
Au <sub>12</sub>			
79	1.50866800	-0.00555400	1.03310000
79	-1.50866800	0.00555400	1.03310000
79	-0.00188600	1.60249500	3.05526500
79	1.54570200	1.37142600	-1.42220900
79	-1.54047100	1.37115300	-1.42993300
79	-0.00235600	2.89902600	0.69643500
79	0.00235600	3.75726600	-1.93265800
79	-0.00235600	-3.75726600	-1.93265800
79	0.00235600	-2.89902600	0.69643500
79	-1.54570200	-1.37142600	-1.42220900
79	0.00188600	-1.60249500	3.05526500
79	1.54047100	-1.37115300	-1.42993300
Au <sub>13</sub>			
79	-0.27211800	3.70815400	0.00000000
79	1.79273800	-0.37464000	1.56194400
79	-0.63513100	-1.71491100	1.56621900
79	-0.63513100	1.14778700	1.49825500
79	-2.93187600	-0.51190700	0.00000000
79	-2.99737600	2.19670500	0.00000000
79	-2.51703400	-3.24672900	0.00000000
79	1.79273800	-0.37464000	-1.56194400

79	-0.63513100	1.14778700	-1.49825500
79	-0.63513100	-1.71491100	-1.56621900
79	4.09022400	0.41732700	0.00000000
79	1.59554200	-2.89399000	0.00000000
79	1.98768700	2.21396800	0.00000000

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Au<sub>14</sub>  
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79	-0.00323000	3.98685000	0.00391400
79	3.85562200	-0.06945900	-0.00128400
79	-0.00769300	1.63736300	1.69547900
79	0.00277900	1.64131200	-1.69677200
79	1.40352700	-0.72462500	-1.53101700
79	1.40470900	-0.72195200	1.52899900
79	-2.36475100	2.23011100	-0.00553100
79	2.79745300	-2.82422100	0.00157200
79	-1.40288300	-0.72185300	-1.52622200
79	-1.40088500	-0.73277000	1.53115400
79	0.00238900	-3.02766200	-0.00447900
79	-3.85379800	-0.07573200	0.00038600
79	-2.79316500	-2.82938500	-0.00051600
79	2.35992400	2.23202200	0.00431600

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Au<sub>15</sub>  
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79	0.00000000	2.53780300	-2.67538700
79	-1.58007100	-1.40678700	-0.35988400
79	1.47245200	-0.00000000	-2.91524300
79	-1.58007100	1.40678700	-0.35988400
79	0.00000000	-3.83302000	-0.04930600
79	1.58007100	-1.40678700	-0.35988400
79	-1.98795200	0.00000000	2.04220000
79	1.58007100	1.40678700	-0.35988400
79	0.00000000	3.83302000	-0.04930600
79	0.00000000	-2.21013700	2.23897800
79	0.00000000	2.21013700	2.23897800
79	1.98795200	-0.00000000	2.04220000
79	-0.00000000	0.00000000	4.15705500
79	-1.47245200	0.00000000	-2.91524300
79	-0.00000000	-2.53780300	-2.67538700

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Au<sub>16</sub>  
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79	1.91760800	0.87118000	2.17974500
79	1.61464500	3.20397600	0.39741600
79	-4.05297300	-0.94521400	-1.11369600
79	-1.24061400	-0.97899300	-1.50815700
79	-2.39057200	-2.88376500	0.48183300
79	0.35296300	-3.33260600	0.08630600
79	1.49855400	-1.03484200	-1.78228800
79	-2.77681800	1.53011100	-1.03361800
79	-2.85730600	-0.27168100	1.67719000
79	0.21251700	1.41720100	-1.46645500
79	-0.15974500	-1.04294500	1.76105300
79	4.25954700	-1.39755800	-1.26427300
79	2.55837700	-1.69513900	1.08348500
79	3.15687100	1.03346300	-0.47070700
79	-0.93356600	1.70042200	1.44884200
79	-1.15948700	3.82638800	-0.47667700

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Au<sub>17</sub>  
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79	-1.12065700	3.69420500	-0.00045400
79	-1.12058800	-3.69418600	0.00027100
79	0.82056300	-2.14494800	1.50176400

79	0.82171600	-2.14641200	-1.50196900
79	3.21238700	-1.66920500	0.00071200
79	-2.02635600	-1.43287400	1.53030900
79	-2.02492000	-1.43272200	-1.52957500
79	2.55819100	0.00028600	2.29805600
79	2.55887800	-0.00025000	-2.29707700
79	-0.22556700	0.00046000	3.25087200
79	-0.22437500	-0.00036000	-3.25084800
79	3.21239900	1.66917500	0.00032600
79	-4.03251600	-0.00008900	-0.00078000
79	-2.02586600	1.43271500	1.52911900
79	-2.02551700	1.43280600	-1.53065600
79	0.82089200	2.14588700	1.50176900
79	0.82133800	2.14551200	-1.50184100

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Au<sub>18</sub>  
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79	-1.60100500	-2.09922800	2.47027000
79	1.08946100	-2.32925600	-1.58443900
79	2.45145400	0.30825800	-1.47718200
79	-1.19383800	-3.36937900	0.00000000
79	0.17060200	2.14064700	1.89704900
79	2.37608000	2.72614900	-0.00000000
79	-2.31359100	0.72850100	2.49702100
79	-2.61627800	-0.74746900	0.00000000
79	0.44336800	-0.19719100	-3.45138700
79	-1.60100500	-2.09922800	-2.47027000
79	0.17060200	2.14064700	-1.89704900
79	-2.15308200	2.08794200	0.00000000
79	-0.31617000	4.23392500	0.00000000
79	-2.31359100	0.72850100	-2.49702100
79	1.08946100	-2.32925600	1.58443900
79	2.45145400	0.30825800	1.47718200
79	0.44336800	-0.19719100	3.45138700
79	3.42271100	-2.03463200	-0.00000000

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Au<sub>19</sub>  
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79	-1.91035700	2.24259100	-1.56229900
79	-3.80504200	-2.98369200	-1.44818900
79	-0.68365400	4.78661200	-1.44824300
79	-1.78229200	0.71629400	0.93394600
79	-2.68363000	-2.10485700	0.99504400
79	-0.00030900	-0.00021100	-1.71949100
79	-0.98758200	-2.77527400	-1.56303000
79	-0.48102200	3.37602500	0.99477400
79	1.20699600	2.68645800	-1.56321300
79	-1.36835000	-1.07456300	3.22001800
79	0.27080400	-1.90177400	0.93318600
79	-0.24447700	1.72180600	3.21932100
79	1.51409400	1.18671600	0.93374500
79	1.72250000	-2.38841800	-1.56402500
79	2.89728000	0.53288800	-1.56317800
79	1.61490500	-0.64875300	3.21900500
79	3.16474000	-1.27192000	0.99421100
79	4.48636600	-1.80265700	-1.44944400
79	-2.93097000	-0.29727100	-1.56213800

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Au<sub>1</sub>  
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79	0.00000000	0.00000000	0.00000000
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Au<sub>20</sub>  
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79	0.00000000	-4.18617200	2.95978000
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79	0.0000000	4.18617200	2.95978000
79	1.57551100	2.94257900	0.96716500
79	2.94257900	1.57551100	-0.96716500
79	-1.57551100	2.94257900	0.96716500
79	0.0000000	1.36734700	3.19344200
79	1.63766100	-0.0000000	1.15722200
79	0.0000000	1.63766100	-1.15722200
79	4.18617200	-0.0000000	-2.95978000
79	-1.63766100	-0.0000000	1.15722200
79	-2.94257900	1.57551100	-0.96716500
79	1.36734700	-0.0000000	-3.19344200
79	2.94257900	-1.57551100	-0.96716500
79	-0.0000000	-1.36734700	3.19344200
79	-0.0000000	-1.63766100	-1.15722200
79	-1.36734700	0.0000000	-3.19344200
79	1.57551100	-2.94257900	0.96716500
79	-2.94257900	-1.57551100	-0.96716500
79	-1.57551100	-2.94257900	0.96716500
79	-4.18617200	0.0000000	-2.95978000

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Au<sub>2</sub>  
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79	0.0000000	0.0000000	1.29607900
79	0.0000000	0.0000000	-1.29607900

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Au<sub>3</sub>  
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79	0.0000000	0.0000000	0.0000000
79	0.0000000	0.0000000	2.69149200
79	0.0000000	0.0000000	-2.69149200

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Au<sub>4</sub>  
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79	0.0000000	1.35482000	0.0000000
79	0.0000000	0.0000000	2.43828700
79	0.0000000	0.0000000	-2.43828700
79	-0.0000000	-1.35482000	0.0000000

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Au<sub>5</sub>  
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79	-0.0000000	0.0000000	1.07435600
79	0.0000000	1.40243400	-1.48283100
79	0.0000000	2.72220500	0.94565300
79	-0.0000000	-2.72220500	0.94565300
79	-0.0000000	-1.40243400	-1.48283100

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Au<sub>6</sub>  
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79	-0.0000000	1.47131500	0.84937900
79	-0.0000000	0.0000000	3.14030700
79	0.0000000	-2.71969700	-1.57044700
79	0.0000000	-0.0000000	-1.69817000
79	0.0000000	2.71969700	-1.57044700
79	-0.0000000	-1.47131500	0.84937900

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Au<sub>7</sub>  
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79	-0.0000000	1.32671700	0.0000000
79	-2.70593700	1.64985200	0.0000000
79	2.22280700	3.04002500	0.0000000
79	-1.20725000	-3.57179300	0.0000000
79	0.90531700	-1.83010300	0.0000000
79	-1.84324700	-0.91608800	0.0000000
79	2.62831000	0.30139000	0.0000000

Au<sub>8</sub>

79	-0.00472800	2.06115200	-0.00001300
79	2.06210200	0.00472900	0.00002400
79	2.63961900	2.65158500	0.00089800
79	2.65139400	-2.63981100	-0.00090800
79	0.00472800	-2.06115200	-0.00001200
79	-2.06210200	-0.00472900	0.00002300
79	-2.65139400	2.63981100	-0.00091000
79	-2.63961900	-2.65158500	0.00089800

Au<sub>9</sub>

79	1.08101200	-0.00002000	0.00005200
79	2.29112800	2.46978600	0.00001600
79	-2.27749200	0.00001400	-0.00007800
79	-0.48050600	-2.34293700	0.00009300
79	3.93738700	0.00000800	-0.00020600
79	2.29107700	-2.46985000	-0.00001700
79	-3.18109600	-2.57853900	0.00002500
79	-0.48046700	2.34294100	0.00039700
79	-3.18104200	2.57859700	-0.00028200

CH<sub>4</sub>\_Au<sub>10</sub>

79	-4.26016700	-0.00033200	0.03354900
79	1.45529500	-0.00019000	-0.06681900
79	2.83903800	-2.43895800	-0.02478000
79	-1.44797700	-0.00022300	-0.08298600
79	0.00268400	2.43770800	-0.11168800
79	4.26763300	0.00028700	0.04317400
79	2.83832800	2.43894500	-0.02430500
79	-2.83305600	2.43894200	-0.03260600
79	0.00317500	-2.43795000	-0.11148600
79	-2.83279200	-2.43936900	-0.03079600
6	-0.25376400	0.00899300	3.23029900
1	0.26030800	0.89707900	2.84897400
1	-1.29565500	0.02079400	2.89156900
1	0.24149700	-0.88800600	2.84490400
1	-0.22425800	0.00611800	4.32335000

CH<sub>4</sub>\_Au<sub>11</sub>

79	3.69839800	-1.78823400	-0.09349100
79	-1.17239500	-2.66247500	-0.01131900
79	1.48911600	-3.67046200	-0.00508200
79	-2.14683500	2.86842100	-0.07292600
79	2.81983100	3.61775100	0.02613400
79	-4.30588400	1.05780900	0.00794400
79	0.54628500	2.02689100	-0.05005300
79	-1.58360600	0.14345500	-0.06207600
79	3.29257400	0.94823000	-0.05966300
79	-3.81112100	-1.67307100	0.00944400
79	1.04732700	-0.86419800	-0.09994000
6	0.99757500	-0.03249700	3.24826300
1	-0.03905900	0.08560100	2.91805000
1	1.37443800	-1.00702600	2.92015000
1	1.61023300	0.75950100	2.80474700
1	1.04743800	0.03166300	4.33870600

CH<sub>4</sub>\_Au<sub>12</sub>

79	0.08102600	1.09930600	-1.50621200
79	-0.08322800	1.06294200	1.51229400
79	-1.62151500	3.09505400	0.04707300

79	-1.35840100	-1.30726500	-1.59183600
79	-1.37477600	-1.44205200	1.50165700
79	-2.90815500	0.72888500	0.02711400
79	-3.73782000	-1.91449000	-0.06459600
79	3.75930100	-1.87029500	0.02147600
79	2.89005800	0.75807200	-0.01400200
79	1.36316000	-1.34168100	1.55922400
79	1.58634100	3.11710300	0.00045800
79	1.37973900	-1.40702800	-1.52906600
6	0.19189800	-4.57195700	0.28756100
1	-0.48082700	-4.01291400	-0.37242500
1	-0.03732300	-4.32214300	1.32898000
1	0.05643900	-5.64492400	0.12713500
1	1.22766900	-4.29372000	0.06766400

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CH<sub>4</sub>\_Au<sub>13</sub>  
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79	-1.76462100	3.24878000	-0.14132800
79	-1.20817100	-1.31769600	-1.62267400
79	1.55586800	-1.11639800	-1.54538300
79	-0.00344900	1.28220800	-1.54877200
79	2.76558400	1.15660500	0.04681400
79	1.34685100	3.46510400	-0.02253900
79	3.90482600	-1.36340800	0.12109700
79	-1.32188600	-1.28808000	1.49922900
79	-0.11874200	1.31746400	1.44765500
79	1.44027200	-1.07765200	1.59685100
79	-3.62349400	-1.88566500	-0.14119100
79	0.28297300	-3.30171900	0.01377300
79	-2.84035700	0.76483700	-0.15994100
6	-3.28427400	0.91369100	3.60707200
1	-3.07467800	1.78704200	2.98123900
1	-2.34113400	0.50672900	3.98487800
1	-3.92378600	1.20338500	4.44537300
1	-3.79145700	0.15473100	3.00226300

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CH<sub>4</sub>\_Au<sub>14</sub>  
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79	0.89080300	3.83828100	-0.26938100
79	-3.80567800	0.79491600	-0.01353300
79	0.39041300	1.42356000	-1.76442200
79	0.39451200	1.67068200	1.64128700
79	-1.51782700	-0.30566100	1.52540000
79	-1.60182900	-0.47369000	-1.52518500
79	2.82202800	1.63075000	-0.10142200
79	-3.38895900	-2.12285400	0.16595400
79	1.21343100	-0.95395200	1.47106500
79	1.08928500	-1.22963100	-1.59005900
79	-0.72671200	-2.97165500	0.17160200
79	3.68169300	-0.97395500	-0.10831200
79	2.05061400	-3.42835000	0.08952000
79	-1.77765800	2.64584800	-0.13456400
6	2.25869000	3.59988300	3.49188900
1	2.81214700	3.91524800	2.60282800
1	2.36047400	2.51697300	3.61725400
1	2.65840800	4.10479400	4.37558500
1	1.20168600	3.86477400	3.37507000

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CH<sub>4</sub>\_Au<sub>15</sub>  
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79	2.85942500	-2.27482600	-0.18600800
79	0.24418300	1.37890400	1.60486700
79	2.88446000	0.34374600	-1.52686500
79	0.47209100	-1.42029700	1.49699100
79	-0.26936600	3.85144000	0.16296500

79	0.22163200	1.54118300	-1.55352400
79	-2.03361700	-0.23409900	1.97140800
79	0.44410200	-1.26096400	-1.66225100
79	0.34902200	-3.78169300	-0.22617700
79	-2.42191600	2.05347200	0.10390500
79	-2.06213400	-2.35474900	-0.11690900
79	-2.06124600	-0.03187600	-1.99804300
79	-4.15162700	-0.30702200	-0.01204700
79	2.90360700	0.19514300	1.41748600
79	2.45023900	2.77296300	0.06324100
6	1.35215800	-3.72341600	3.64130100
1	0.33646300	-3.88204800	3.26416200
1	1.46007100	-2.68940800	3.98415400
1	1.53724600	-4.40343300	4.47744900
1	2.07367200	-3.91918500	2.84238400

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CH<sub>4</sub>\_Au<sub>16</sub>  
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79	-1.91963000	0.67860000	-2.26686200
79	-1.67404300	3.10245700	-0.60891900
79	4.08338200	-0.80050200	1.14991100
79	1.26525700	-0.89870000	1.52077800
79	2.48987200	-2.86878300	-0.33666000
79	-0.24737400	-3.36470100	0.04563900
79	-1.47002900	-1.01940400	1.78642500
79	2.73773200	1.63386800	0.96096000
79	2.87777100	-0.29846500	-1.66576100
79	-0.24210200	1.45370300	1.39148400
79	0.20890100	-1.15502200	-1.75376300
79	-4.21502400	-1.47243000	1.27193500
79	-2.49068500	-1.84962700	-1.05986000
79	-3.16901000	0.94199400	0.36410100
79	0.89826600	1.62112000	-1.53225500
79	1.05969700	3.85344700	0.27860600
6	-1.52482900	3.49518400	3.58824300
1	-1.84701900	4.00900600	2.67758700
1	-0.43436000	3.38960000	3.58238300
1	-1.82442400	4.07729700	4.46416300
1	-1.99081000	2.50599800	3.63138300

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CH<sub>4</sub>\_Au<sub>17</sub>  
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79	1.60997900	-3.55992500	-0.05406100
79	0.64167600	3.77012200	0.05732700
79	-1.07356900	1.95712600	1.54165100
79	-1.08542200	1.99725700	-1.47003300
79	-3.39362100	1.23314700	0.03525700
79	1.83532900	1.62393600	1.53722100
79	1.82284600	1.66673100	-1.50375900
79	-2.51429800	-0.41355000	2.27623900
79	-2.53586100	-0.34925000	-2.25958700
79	0.25150200	-0.06239600	3.25129900
79	0.22126400	0.03122900	-3.24805100
79	-2.94553100	-2.15962900	-0.01569800
79	4.01649900	0.48271200	-0.00964100
79	2.22357300	-1.21536600	1.50795200
79	2.20720600	-1.17360600	-1.55524400
79	-0.50211200	-2.29298000	1.47347300
79	-0.51685200	-2.25548100	-1.53434700
6	-2.07494200	5.68770600	-0.23711300
1	-2.60156700	4.76776200	0.03228500
1	-1.33966800	5.92431700	0.54017100
1	-1.56820100	5.54254700	-1.19687900
1	-2.78700800	6.51299700	-0.32292300

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CH<sub>4</sub>\_Au<sub>18</sub>

79	1.89298400	-2.40807900	-1.94777200
79	2.43376200	1.16523700	1.31539300
79	-0.21863700	1.07616300	2.63866900
79	3.36059800	-0.14887300	-1.17922700
79	-2.29237400	-1.74463500	-0.10271600
79	-2.74768500	-0.17397000	2.37546300
79	-0.91572900	-2.09826400	-2.65880600
79	0.76557900	0.28266300	-2.59228500
79	0.46076900	3.27310400	0.96772900
79	2.30567100	2.44915500	-1.21265400
79	-1.98585700	1.96732900	0.44992500
79	-2.06884200	0.45457200	-2.13414400
79	-4.22478900	0.35260900	-0.30907500
79	-0.49728100	2.82246700	-1.90944200
79	2.17597800	-1.96499700	0.84746800
79	-0.45875500	-1.83921800	2.21244200
79	-0.10800900	-3.52265000	-0.06910400
79	1.97534700	-0.72278700	3.39273600
6	1.16301300	6.16376800	-0.66840500
1	0.09657100	5.92539900	-0.72881100
1	1.53992000	5.91987000	0.33083200
1	1.70803100	5.57612600	-1.41404600
1	1.31166500	7.22966700	-0.86104400

CH<sub>4</sub>\_Au<sub>19</sub>

79	2.62699000	-1.37145100	-1.49045500
79	2.42107000	4.18241500	-1.42127000
79	2.43423400	-4.18687600	-1.37493700
79	1.91188200	0.01149800	0.98368500
79	1.68530500	2.96842200	1.03112500
79	0.01290600	-0.00634800	-1.65600600
79	-0.10952200	2.93418100	-1.55167100
79	1.69626200	-2.94765800	1.06524700
79	-0.10110600	-2.94904200	-1.51910900
79	0.83052600	1.52643900	3.25096100
79	-0.97764200	1.67252600	0.94608100
79	0.83439000	-1.48360100	3.26745600
79	-0.97197800	-1.66313700	0.96373500
79	-2.47812000	1.56172500	-1.56857900
79	-2.47480500	-1.58673600	-1.54720800
79	-1.77299500	0.01629600	3.23332900
79	-3.42550800	0.00289400	0.99581700
79	-4.82143700	-0.01488000	-1.46866100
79	2.62289300	1.36513800	-1.50998800
6	0.44764500	-0.25139800	-4.97448900
1	-0.41225500	-0.83175500	-4.62557700
1	0.35126000	0.78353200	-4.63089300
1	1.36522000	-0.68369900	-4.56399600
1	0.48556600	-0.27226400	-6.06727600

CH<sub>4</sub>\_Au<sub>1</sub>

6	2.98657700	0.00000100	0.00002100
1	2.61929500	1.01728500	-0.16474200
1	2.61851500	-0.65435800	-0.79569800
1	4.07973200	0.00208200	-0.00688300
1	2.62890900	-0.36503000	0.96723000
79	-0.37805000	0.00000000	-0.00000000

CH<sub>4</sub>\_Au<sub>20</sub>

79	-0.98861900	-4.34559200	-2.52145100
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79	-1.05402500	4.01202400	-3.00100600
79	-1.80056700	2.90975400	-0.50609000
79	-2.37986900	1.66979700	1.85870000
79	1.13997300	2.85986300	-1.63474000
79	-1.12079200	1.18557800	-3.05403900
79	-1.90344100	-0.04326600	-0.49981600
79	0.43232800	1.70326900	0.98766400
79	-2.83042800	0.22224900	4.24336500
79	1.15240300	-0.08700700	-1.66361100
79	3.11551300	1.58717600	-0.23648300
79	-0.10503700	0.19827900	3.46822400
79	-2.35598800	-1.48238400	2.03918900
79	-1.09967600	-1.54523100	-2.89646900
79	0.45738900	-1.57236100	1.17582000
79	2.44769900	0.16160100	2.49263100
79	-1.75506100	-2.97504300	-0.16933800
79	3.14002600	-1.55636500	-0.05522400
79	1.18602400	-3.01137500	-1.29699800
79	4.99954300	0.11144100	1.26909900
6	-5.35277900	-0.01900600	0.00402300
1	-6.43482100	-0.03701900	-0.15368900
1	-4.90390500	-0.92469800	-0.41593600
1	-4.92327900	0.86069900	-0.48553200
1	-5.13553800	0.02504500	1.07635500

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CH<sub>4</sub>\_Au<sub>2</sub>  
-----

79	-1.03957200	-0.00038300	0.00431200
79	1.53623400	0.00020100	-0.00227100
6	-3.92120600	0.00142500	-0.01669700
1	-4.60171100	-0.00262900	0.83686700
1	-3.31273900	0.91675000	0.03360200
1	-3.31521600	-0.91599900	0.02292600
1	-4.47936100	0.00764300	-0.95442400

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CH<sub>4</sub>\_Au<sub>3</sub>  
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79	-1.30738700	-0.07606200	-0.00018400
79	0.98528900	-1.48947600	0.00013400
79	0.85114500	1.57261600	-0.00003300
6	-4.17647600	-0.05594000	0.00071400
1	-4.79865500	0.18367300	-0.86325400
1	-3.57833600	-0.94769300	-0.24232300
1	-3.56369800	0.82722400	0.23831900
1	-4.79521400	-0.28668100	0.86952700

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CH<sub>4</sub>\_Au<sub>4</sub>  
-----

79	-0.00000500	1.24134900	0.00009800
79	-2.44817700	-0.15360500	-0.00002600
79	2.44822800	-0.15332500	-0.00002600
79	0.00008700	-1.45193400	-0.00001000
6	-0.00106800	4.08579500	-0.00028000
1	0.89674800	4.70585200	0.00084100
1	-0.90046600	4.70354100	-0.00172800
1	0.00111500	3.47947100	-0.91980000
1	-0.00152200	3.47995900	0.91956900

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CH<sub>4</sub>\_Au<sub>5</sub>  
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79	0.00089600	-1.08910100	-0.03948000
79	-1.40137900	1.46850200	-0.12965400
79	-2.72114600	-0.95887400	-0.06086000
79	2.72289800	-0.95798700	-0.05647500
79	1.40243400	1.46899000	-0.12929900

6	-0.02926100	0.54069500	3.28637200
1	-0.00855100	0.51084200	4.37908300
1	0.85015900	0.02724000	2.88485800
1	-0.93440000	0.04640100	2.91951000
1	-0.02404700	1.58044300	2.94397900

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CH<sub>4</sub>\_Au<sub>6</sub>  
-----

79	1.14646100	1.25380500	-0.06153700
79	-0.94751800	2.99340700	-0.07746400
79	-2.11919300	-2.31717200	-0.07482100
79	0.51334000	-1.62106600	-0.06304100
79	3.06669200	-0.67603500	-0.07563100
79	-1.65921600	0.36541500	-0.06312700
6	-0.00444800	0.01300500	3.28493200
1	-0.00459500	0.01196400	4.37835300
1	-0.36403100	0.97892100	2.91638100
1	1.01157900	-0.15837000	2.91553000
1	-0.66095800	-0.78052900	2.91418300

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CH<sub>4</sub>\_Au<sub>7</sub>  
-----

79	-1.12491700	0.76434000	-0.04787400
79	0.14777200	3.17324100	-0.09281600
79	-3.76568900	-0.15792400	0.01040500
79	3.63386100	-0.98919100	-0.03422500
79	1.01786300	-1.78992300	-0.08127100
79	1.76942900	1.00673600	-0.05308200
79	-1.71323400	-2.00345100	-0.10942700
6	0.27583200	-0.03007700	3.22692600
1	-0.51417900	-0.63177100	2.76508800
1	1.25030300	-0.39610400	2.88812600
1	0.15808800	1.01524500	2.92462300
1	0.20905500	-0.10935300	4.31545200

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CH<sub>4</sub>\_Au<sub>8</sub>  
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79	-2.05909000	0.11248600	-0.05702100
79	-0.10578600	-2.05394500	-0.04126400
79	-2.77716900	-2.49805300	-0.12682800
79	2.50237500	-2.78497400	0.01841000
79	2.07529400	-0.11159100	-0.04804000
79	0.11773300	2.05130500	-0.03510700
79	-2.48982300	2.78652400	-0.00995000
79	2.78974200	2.49963000	-0.09807800
6	-0.42148000	-0.01086700	3.14461700
1	-1.03494800	-0.88485000	2.90401400
1	0.49961900	-0.04224100	2.55103500
1	-0.97577000	0.90084700	2.90101900
1	-0.16877200	-0.01776400	4.20852700

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CH<sub>4</sub>\_Au<sub>9</sub>  
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79	1.08581400	0.00486500	-0.04215400
79	2.29546200	-2.46584100	-0.06181300
79	-2.27102200	0.00498000	-0.03917900
79	-0.47367900	2.35263900	-0.05731000
79	3.93950000	0.00224100	-0.00338000
79	2.29515800	2.47405100	-0.03642500
79	-3.17369300	2.58333100	-0.03939200
79	-0.47330100	-2.34383900	-0.06806000
79	-3.17375500	-2.57339400	-0.05401500
6	-0.39875700	-0.30850400	3.17468900
1	0.57632900	-0.73256900	2.91353600
1	-1.18954200	-0.98333800	2.83140400

1	-0.46663800	-0.18114600	4.25862600
1	-0.51580200	0.66448000	2.68479700

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CH<sub>4</sub>  
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6	0.00000000	0.00000000	0.00000000
1	0.63064700	0.63064700	0.63064700
1	-0.63064700	-0.63064700	0.63064700
1	-0.63064700	0.63064700	-0.63064700
1	0.63064700	-0.63064700	-0.63064700

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CO<sub>2</sub>\_Au<sub>10</sub>  
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79	4.26506500	-0.00000700	-0.01850600
79	-1.45601800	0.00008400	-0.14110500
79	-2.83995000	2.43955500	-0.07644400
79	1.45566600	0.00013200	-0.14141100
79	0.00002200	-2.43050700	-0.10993500
79	-4.26475500	0.00010300	-0.01834400
79	-2.83998400	-2.43934000	-0.07648300
79	2.83984400	-2.43899300	-0.07670200
79	-0.00001600	2.43072300	-0.10932100
79	2.83983000	2.43915700	-0.07619100
6	0.00106100	-0.00327300	3.02880900
8	1.18620800	-0.00078200	3.03397200
8	-1.18408700	-0.00570600	3.03329600

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CO<sub>2</sub>\_Au<sub>11</sub>  
-----

79	3.72054500	-1.78284400	-0.04756000
79	-1.14536800	-2.67520500	-0.07091000
79	1.52339000	-3.67417400	-0.03345800
79	-2.14070100	2.85225600	-0.10927200
79	2.81709200	3.62424900	-0.05741200
79	-4.28929200	1.03500600	-0.03807400
79	0.55484100	2.01797500	-0.12165600
79	-1.56669000	0.12731500	-0.13697800
79	3.30367400	0.95544800	-0.04345700
79	-3.78551800	-1.69494600	-0.06239100
79	1.06960000	-0.86920100	-0.11984000
6	-0.22149300	0.30263900	3.01605000
8	0.94871700	0.12054700	2.96074800
8	-1.39063300	0.48316700	3.08217900

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CO<sub>2</sub>\_Au<sub>12</sub>  
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79	-0.02478200	1.03023600	1.40261200
79	-0.02010900	1.06340200	-1.59844700
79	1.57266400	3.07488300	-0.08258300
79	1.38276600	-1.43251400	1.39480000
79	1.35108700	-1.39776300	-1.69920500
79	2.87314600	0.71856900	-0.12965300
79	3.75349000	-1.90089300	-0.18011800
79	-3.75210500	-1.94958800	-0.09089200
79	-2.90489700	0.68012100	-0.03833400
79	-1.39089200	-1.39673800	-1.65852400
79	-1.63650400	3.05552500	-0.03147300
79	-1.34774400	-1.47301200	1.43587800
6	0.51502700	-0.26107900	4.58123400
8	0.16920000	0.85791900	4.39175300
8	0.86535000	-1.37536200	4.77220500

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CO<sub>2</sub>\_Au<sub>13</sub>  
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79	-1.61831900	3.35397500	-0.09701000
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79	-1.44408700	-1.24029000	-1.60391800
79	1.32826600	-1.20949800	-1.69148800
79	-0.08401200	1.28301700	-1.61221100
79	2.77488400	0.99061500	-0.18302600
79	1.50360700	3.38368900	-0.18319700
79	3.76794000	-1.59037600	-0.19008800
79	-1.33600000	-1.19389400	1.53155700
79	0.00294700	1.34054200	1.37152400
79	1.42548700	-1.17287500	1.43774300
79	-3.77360200	-1.66590300	0.04777200
79	0.01360600	-3.31428500	-0.06329200
79	-2.83812700	0.93412100	-0.01634700
6	0.99545900	0.36247300	4.49887600
8	0.47367400	1.41348400	4.32560500
8	1.51915400	-0.68635100	4.66355400

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CO<sub>2</sub>\_Au<sub>14</sub>  
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79	-0.01798500	3.99578700	0.03195400
79	3.85493900	-0.04103100	-0.08154800
79	-0.01311300	1.57412900	1.62484400
79	-0.01216700	1.72773700	-1.76794200
79	1.40686600	-0.62969200	-1.62900000
79	1.40888900	-0.77776700	1.41914200
79	-2.37432800	2.23261300	-0.04724000
79	2.80648400	-2.79807500	-0.18131000
79	-1.40482400	-0.64592400	-1.62259100
79	-1.39759700	-0.79593600	1.43550700
79	0.01203000	-3.00924100	-0.18670600
79	-3.85314200	-0.07907600	-0.06772600
79	-2.78445700	-2.82628800	-0.16976600
79	2.34580500	2.25104400	-0.04007000
6	0.08120000	-0.63889900	4.60420800
8	-1.10102300	-0.56996300	4.65109500
8	1.26329300	-0.71139000	4.55995700

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CO<sub>2</sub>\_Au<sub>15</sub>  
-----

79	2.66852200	2.53672500	-0.14736400
79	0.25873200	-1.40982800	-1.71606200
79	2.99352600	0.00081200	1.31346000
79	0.25930900	1.40470200	-1.71089300
79	0.03626300	-3.83032400	-0.10695000
79	0.41702000	-1.39703000	1.43346600
79	-2.17732200	-0.00190100	-2.01249800
79	0.41894200	1.40273200	1.43934400
79	0.03803600	3.83019100	-0.11286900
79	-2.24934500	-2.20493600	-0.01625000
79	-2.24862800	2.20603200	-0.02164700
79	-1.95110000	0.00330800	1.99191900
79	-4.15716800	0.00038200	0.12518300
79	2.79655300	-0.00238100	-1.62092200
79	2.66766100	-2.53798600	-0.14291200
6	0.82133100	-0.00175300	4.68448700
8	-0.33150000	0.00135200	4.95506400
8	1.97687100	-0.00497100	4.41838700

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CO<sub>2</sub>\_Au<sub>16</sub>  
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79	1.96664500	0.80805000	2.22110600
79	1.64939200	3.19556100	0.51123600
79	-4.03074300	-0.94256900	-0.98996800
79	-1.23001100	-0.96695300	-1.40594600
79	-2.34573200	-2.91020200	0.57577500
79	0.38284800	-3.34377900	0.04791500

79	1.49289300	-0.99028700	-1.79691400
79	-2.77538700	1.52499400	-0.84691100
79	-2.79903700	-0.34781600	1.85867800
79	0.22213200	1.44384500	-1.34343500
79	-0.09848900	-1.11233500	1.81725700
79	4.26702700	-1.35758600	-1.32239600
79	2.59859500	-1.71991300	1.02853700
79	3.17563600	1.04945300	-0.44125200
79	-0.89161800	1.64301200	1.57545300
79	-1.15756800	3.81474400	-0.28012800
6	-1.53211100	0.75864900	-4.33903000
8	-1.32612100	1.88593500	-4.03149900
8	-1.73728200	-0.36359500	-4.65319500

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CO<sub>2</sub>\_Au<sub>17</sub>  
-----

79	-1.95875800	-3.25179300	-0.98659100
79	-0.35342200	3.73238700	0.80990700
79	1.41660000	2.09155400	-0.79574000
79	0.93329400	1.46804200	2.09371800
79	3.38669900	0.75736300	0.79846200
79	-1.46194100	2.13987400	-1.31953200
79	-1.96354200	1.49757900	1.63411000
79	2.76609000	-0.22508400	-1.87211300
79	2.01044400	-1.16845700	2.51000800
79	0.26480200	0.69594600	-3.11533200
79	-0.81590400	-0.66645500	3.14532900
79	2.64459700	-2.46978300	-0.01867200
79	-3.95351000	0.96399500	-0.41060800
79	-2.08003700	-0.56642100	-2.01839400
79	-2.58539300	-1.20588800	0.94101200
79	0.49326800	-1.96368200	-1.84295900
79	-0.00845900	-2.59647200	1.05564600
6	4.54468100	2.75633000	-2.18289600
8	3.87741200	3.70594400	-1.94513100
8	5.20765300	1.80382900	-2.42416300

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CO<sub>2</sub>\_Au<sub>18</sub>  
-----

79	2.42327000	-1.17516400	2.47770900
79	2.06423500	1.47307800	-1.59099600
79	-0.79793200	2.23856500	-1.49856900
79	3.58268900	-0.50763000	0.00889900
79	-2.09237200	-0.37035600	1.88928400
79	-3.14275500	1.66183500	-0.01588700
79	-0.17580700	-2.48956600	2.50878900
79	1.33033400	-2.47532700	0.01584600
79	0.12840800	0.37995800	-3.45741200
79	2.43192400	-1.20728300	-2.45466400
79	-2.08432700	-0.39084500	-1.89032600
79	-1.53824600	-2.63784400	0.01211500
79	-4.02946900	-1.31370000	0.00026200
79	-0.16878300	-2.51618200	-2.48444400
79	2.05922300	1.49266800	1.58185100
79	-0.80290800	2.25434200	1.46785100
79	0.11487700	0.41905100	3.45353800
79	1.27440700	3.70521100	-0.01771300
6	-2.07406500	5.23829500	-0.02207700
8	-2.13819600	5.23355600	1.16104500
8	-2.00183100	5.24723500	-1.20503800

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CO<sub>2</sub>\_Au<sub>19</sub>  
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79	-2.59673200	-1.57107500	-1.25364100
79	2.28943100	-4.18941400	-1.61120100

79	-4.91700700	0.00575500	-0.92083100
79	-0.83626700	-1.65951200	1.08890300
79	1.81461000	-2.95902000	0.89429400
79	-0.11725800	-0.00013300	-1.62184000
79	2.48341600	-1.37242600	-1.73783900
79	-3.27602100	0.00396500	1.37345300
79	-2.59298000	1.57698000	-1.25413400
79	1.20541300	-1.50441400	3.18775200
79	2.03561600	-0.00229300	0.80812500
79	-1.40176500	0.00201000	3.43279800
79	-0.83234300	1.66176100	1.08836600
79	2.48641300	1.36698900	-1.73765300
79	-0.23321000	2.93971700	-1.48572200
79	1.20868800	1.50090900	3.18782000
79	1.82177000	2.95486300	0.89498800
79	2.29932800	4.18417800	-1.61082600
79	-0.24042000	-2.93968600	-1.48505300
6	-2.15701200	0.00303800	-4.44645500
8	-3.33209700	0.00364700	-4.29394700
8	-0.98189300	0.00242900	-4.59408100

-----  
CO<sub>2</sub>\_Au<sub>1</sub>  
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6	-0.00009600	2.56456600	-0.00000000
8	1.18582300	2.54949500	-0.00000000
8	-1.18575100	2.58632300	-0.00000000
79	-0.00000000	-0.71486000	0.00000000

-----  
CO<sub>2</sub>\_Au<sub>20</sub>  
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79	3.19042700	3.93746200	0.33609000
79	0.71471600	-2.48885500	-4.41041300
79	0.76371400	-2.95916200	-1.62162900
79	0.75861100	-3.18857600	1.10541800
79	-1.33250300	-1.08813700	-3.04961000
79	1.71195800	-0.27085200	-2.97031300
79	1.79041700	-0.69147200	-0.05478800
79	-1.34895800	-1.54415800	-0.13262400
79	0.70413000	-3.19266800	3.93322700
79	-0.37644200	1.25492600	-1.53749100
79	-3.16260100	0.29203000	-1.55826800
79	-1.33988200	-1.58384800	2.82071200
79	1.70387300	-0.76404400	2.88796100
79	2.51630500	1.83124200	-1.42270300
79	-0.38436200	0.97740400	1.72321800
79	-3.16781200	0.02820500	1.58122600
79	2.50925600	1.56680900	1.71308900
79	-2.22671300	2.71631100	0.22323800
79	0.41507300	3.43217500	0.28919000
79	-4.88666100	1.75169600	0.14137600
6	5.19880400	-0.05968000	0.01107100
8	5.56210600	1.06374000	0.10912700
8	4.83242400	-1.18180900	-0.08689600

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CO<sub>2</sub>\_Au<sub>2</sub>  
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79	0.75991300	1.12411900	-0.00000000
79	0.00000000	-1.35653400	0.00000000
6	-2.72461500	0.83333100	-0.00000000
8	-2.38593700	1.96958400	-0.00000000
8	-3.07474000	-0.29948400	0.00000000

-----  
CO<sub>2</sub>\_Au<sub>3</sub>  
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79	0.00000000	0.75240500	-0.00000000
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79	2.58367200	0.01381600	0.00000000
79	-2.58330400	0.01373800	-0.00000000
6	-0.00132500	-2.79779200	-0.00000000
8	1.18417200	-2.80136000	0.00000000
8	-1.18681300	-2.80239800	-0.00000000

-----  
CO<sub>2</sub>\_Au<sub>4</sub>  
-----

79	0.00557400	-1.35962100	-0.23447600
79	2.43978100	0.00026500	-0.15839600
79	-2.43042400	0.00001500	-0.18400300
79	0.00509100	1.35988300	-0.23345200
6	-0.07224800	-0.00194100	2.90860500
8	-0.07173800	1.18356800	2.91147000
8	-0.07178800	-1.18746100	2.90905500

-----  
CO<sub>2</sub>\_Au<sub>5</sub>  
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79	-0.00024100	-1.07827300	-0.22242200
79	-1.40127200	1.48471900	-0.16722800
79	-2.72006500	-0.94432600	-0.14029800
79	2.71948800	-0.94501800	-0.14065400
79	1.40168500	1.48476000	-0.16745100
6	0.00145600	-0.00691500	3.00529600
8	0.00315100	1.17891900	2.99953800
8	-0.00024500	-1.19211000	3.02226100

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CO<sub>2</sub>\_Au<sub>6</sub>  
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79	1.64405600	0.00534800	-0.31023200
79	1.51152800	2.71718900	-0.18259400
79	-3.19386200	-0.00829600	0.00351100
79	-0.90029700	-1.46996000	-0.07285200
79	1.52639900	-2.70743900	-0.18561400
79	-0.90807400	1.46565400	-0.07128100
6	1.15028500	-0.00897900	2.93673300
8	2.33492900	-0.00633200	2.97758300
8	-0.03516700	-0.01157900	2.90811400

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CO<sub>2</sub>\_Au<sub>7</sub>  
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79	1.11859000	0.73606200	-0.08643700
79	-0.19156700	3.12942000	-0.18404400
79	3.80368000	-0.06141300	-0.03925900
79	-3.55926900	-1.12059600	-0.16549300
79	-0.91149500	-1.81627700	-0.07797600
79	-1.78329000	0.94610500	-0.26552000
79	1.82245800	-1.99386500	-0.00609700
6	-1.07509700	0.64824700	2.95778100
8	-2.10448700	1.22056100	3.08708600
8	-0.04287700	0.07632500	2.83973600

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CO<sub>2</sub>\_Au<sub>8</sub>  
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79	-1.46578400	-1.45077000	-0.11756700
79	1.45634000	-1.45997200	-0.11538900
79	-0.01207400	-3.41263200	1.06259100
79	3.45500500	-0.01231400	-1.23562300
79	1.46751300	1.44936800	-0.11412900
79	-1.45490100	1.45931900	-0.11716900
79	-3.45320500	0.01143100	-1.23845600
79	0.01089500	3.41401000	1.05974300
6	-0.01367100	0.00557200	2.92445200
8	-1.19912100	0.00753800	2.94248200
8	1.17195900	0.00369200	2.92216900

CO <sub>2</sub> _Au <sub>9</sub>			
79	1.08435300	0.00020100	-0.46945000
79	2.26383100	-2.45916400	-0.13402300
79	-2.33090000	-0.00006800	0.01692800
79	-0.50404800	2.31046900	-0.11989800
79	3.89895600	0.00034100	0.13589500
79	2.26332300	2.45952500	-0.13507200
79	-3.19335600	2.59156200	0.02152500
79	-0.50359000	-2.31045200	-0.11974500
79	-3.19283500	-2.59206100	0.01996000
6	0.77018000	-0.00127800	2.81114100
8	1.94467300	-0.00198500	2.96902300
8	-0.40642500	-0.00053500	2.66344900

CO <sub>2</sub>			
6	0.00000000	0.00000000	0.00000000
8	0.00000000	0.00000000	1.18539100
8	0.00000000	0.00000000	-1.18539100

CO_Au <sub>10</sub>			
79	4.28108900	0.00000900	-0.05201100
79	-1.44307300	-0.00006800	0.06207200
79	-2.82835700	2.44166800	-0.10350200
79	1.46413000	-0.00002900	-0.04400900
79	0.01132500	-2.43625800	-0.08369800
79	-4.25328200	0.00007300	-0.09256700
79	-2.82844900	-2.44163800	-0.10401400
79	2.84922300	-2.43767600	-0.04426900
79	0.01134800	2.43624300	-0.08365200
79	2.84924100	2.43766700	-0.04483900
6	-1.10669800	-0.00010100	2.86604300
8	-0.28778100	0.00016100	3.68154000

CO_Au <sub>11</sub>			
79	3.68054200	-1.79452600	-0.10229600
79	-1.19162200	-2.65847000	-0.03566700
79	1.46891800	-3.67254100	-0.00129900
79	-2.14441500	2.87587300	-0.06342100
79	2.82152000	3.61338000	-0.02396400
79	-4.30406900	1.07039200	0.03561800
79	0.54550700	2.02596200	-0.03165000
79	-1.58832800	0.14712600	-0.06762500
79	3.28400700	0.94274700	-0.07932300
79	-3.82770300	-1.66290900	-0.01699900
79	1.03263500	-0.86772600	-0.17209400
6	1.23646200	0.50318800	2.90475600
8	1.27485400	-0.56805400	3.33880100

CO_Au <sub>12</sub>			
79	-0.36126600	1.03538700	1.52238000
79	0.22727100	0.97895000	-1.48088100
79	1.44928000	3.19616600	-0.23958300
79	1.29599700	-1.25000100	1.54346000
79	1.31978400	-1.51579200	-1.94584400
79	2.80633800	0.86718700	0.12045100
79	3.98349200	-1.47979100	0.80984600
79	-3.72843600	-2.06674000	-0.06047300
79	-3.08171900	0.62769600	0.08386600
79	-1.36065800	-1.23772100	-1.46180000



79	-1.74213200	2.96810200	-0.04571400
79	-1.41896700	-1.57482000	1.59621300
6	2.94049000	-2.70153400	-2.35264400
8	3.82841800	-3.39151100	-2.59946600

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CO\_Au13

79	0.08449500	3.59065500	0.00596600
79	1.82772700	-0.57306900	2.13766100
79	-0.48167700	-1.74851800	1.27311000
79	-0.33796300	1.07882900	1.36934600
79	-3.01390900	-0.23264000	0.44711400
79	-2.79433000	2.49279100	0.40147900
79	-2.84846700	-2.99269200	0.18425300
79	1.18008000	-0.28035600	-1.99499300
79	-1.09785800	1.24066100	-1.59766700
79	-1.23995900	-1.57022600	-1.69699900
79	3.81396700	-0.35239900	-0.87176900
79	1.97642400	-2.46045400	-0.12450100
79	2.19120400	1.81355100	-0.12886600
6	3.61362400	-0.18068500	3.05503000
8	4.59989900	0.07493800	3.59290300

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CO\_Au14

79	2.82591200	-2.77681700	0.29910600
79	2.14276000	2.14936300	-0.15720800
79	1.40703200	-1.12605800	-1.62682900
79	1.37853400	-0.38777500	1.36590000
79	-0.02220600	1.84838400	2.17322300
79	-0.02196100	1.21507100	-1.97198300
79	0.03975200	-3.01630800	0.46519000
79	-0.04918000	3.84010800	-0.79787600
79	-1.36296200	-0.42347800	1.36188700
79	-1.37861900	-1.16817600	-1.63044800
79	-2.20120300	2.09908500	-0.15077200
79	-2.75296300	-2.84861100	0.30323600
79	-3.81838600	-0.13098900	-0.10987900
79	3.82364000	-0.03354600	-0.11226000
6	-0.04798900	3.69628100	3.03217900
8	-0.06423200	4.73028200	3.53942200

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CO\_Au15

79	2.80328300	2.57211600	-0.36917200
79	-0.39626500	-1.37843000	-1.89907500
79	3.46054100	-0.00738200	0.98340900
79	-0.39546300	1.38053800	-1.90394400
79	-0.02269300	-3.76070100	-0.25300800
79	0.77662900	-1.38906400	1.23851100
79	-2.99540800	0.00292100	-1.59012300
79	0.78052700	1.38612500	1.23808100
79	-0.01204000	3.75918700	-0.25235000
79	-2.20324100	-2.13467500	0.33157800
79	-2.19664900	2.13903200	0.33076400
79	-1.39068000	0.00141900	2.31755500
79	-4.00703500	0.00612900	1.15033800
79	2.07527300	0.00210800	-1.47785700
79	2.78978500	-2.57688200	-0.37801200
6	4.85042800	-0.01204600	2.49954600
8	5.57986200	-0.01505800	3.39173600

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CO\_Au16

79	2.66752800	2.00776300	2.27352100
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79	1.08859900	2.40523200	-0.16398300
79	-3.42198100	-0.70931700	-0.49605100
79	-0.68071400	-1.74827000	-1.02625000
79	-2.68126700	-3.32447500	0.46734100
79	0.24289600	-3.31064500	1.18789700
79	1.32791000	-0.15577700	-2.22459800
79	-3.68165300	1.98382000	-0.96625800
79	-1.84069200	-1.04119200	2.02331800
79	-1.16669800	0.90554900	-1.81074000
79	0.79402500	-0.23110400	1.51955100
79	4.04792700	-0.99107300	-2.07897500
79	2.32988300	-2.26536400	-0.20784600
79	3.26879300	0.59205800	0.09877100
79	-1.48045500	1.55326500	1.24243700
79	-1.26336000	3.73501900	-0.65619300
6	2.56802400	3.02423400	4.04910200
8	2.51043400	3.60261000	5.04151900

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CO\_Au<sub>17</sub>  
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79	3.07860300	2.33504900	0.65868000
79	-3.89520800	0.02830200	-0.62660800
79	-2.20856600	-1.43032700	1.17053500
79	-1.74181200	-1.45960000	-1.92070600
79	-1.23676000	-3.75796800	-0.23204100
79	-2.18246900	1.46114100	1.16569000
79	-1.72070800	1.48513400	-1.92182700
79	0.28264800	-2.51822000	1.95811400
79	0.92514600	-2.11786700	-1.16501200
79	-0.55719800	0.00504100	3.13564200
79	0.53009700	-0.00485000	-3.03126500
79	3.04203800	-2.37950000	0.66127400
79	-1.17975400	3.77638800	-0.23481700
79	0.32084800	2.51607600	1.95981100
79	0.95577300	2.10236200	-1.16475900
79	1.67622200	-0.01107900	1.36250800
79	3.01819200	-0.02035600	-1.22978800
6	4.61314400	-0.04584100	-2.57454200
8	5.35760500	-0.06167300	-3.45521800

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CO\_Au<sub>18</sub>  
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79	-2.97320100	-2.01762400	-0.68861600
79	-1.26420900	2.14199400	0.56507400
79	1.53304400	2.98465400	-0.41355600
79	-3.41377400	0.16887900	1.05155500
79	1.54500600	-1.81975400	-1.70279700
79	3.04123300	0.88721100	-1.83014000
79	-0.50557400	-3.53151800	-0.42562900
79	-1.20598400	-1.75424800	1.72461600
79	0.88226100	2.43967500	2.40966800
79	-1.61179800	0.84370700	3.08055700
79	2.04094600	0.46978600	0.79769800
79	1.54113400	-2.42594200	1.25895300
79	3.87274400	-1.66282500	-0.08897200
79	0.93332400	-0.57823200	3.33020700
79	-2.62973500	0.51811000	-1.79822300
79	0.27981300	0.84101900	-2.15811400
79	-0.97362700	-1.62816800	-2.88509200
79	-1.42705900	3.12641800	-2.03100800
6	1.82690000	4.99068200	-0.94245500
8	1.94245600	6.10096800	-1.23045900

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CO\_Au<sub>19</sub>  
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79	2.78177900	-0.66559300	-1.71061900
79	1.23244100	4.66856800	-1.45224200
79	3.30069400	-3.44173900	-1.65127700
79	1.94422900	0.47173000	0.85686700
79	1.00349100	3.27606500	1.00703100
79	-0.08282900	0.01110400	-1.65040900
79	-0.91469800	2.83627800	-1.43770500
79	2.46524600	-2.44384900	0.86539600
79	0.53676100	-2.86421800	-1.58268700
79	0.67997800	1.64085900	3.23363900
79	-1.26854500	1.36501100	1.05796000
79	1.44672100	-1.26271900	3.17193600
79	-0.43217900	-1.86838900	1.00447800
79	-2.87538600	0.92294800	-1.33761800
79	-2.09345800	-2.13388100	-1.40149300
79	-1.46033900	-0.46256100	3.35984500
79	-3.20947200	-0.86632400	1.24204500
79	-4.74348300	-1.19771000	-1.10639300
79	2.10321800	1.98653400	-1.64573000
6	-2.83411500	0.42654900	-4.30225700
8	-1.96436300	-0.04453600	-4.90067300

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CO\_Au<sub>1</sub>  
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6	0.35905200	-1.73798100	-0.00000000
8	-0.26928900	-2.71793800	-0.00000000
79	-0.00000000	0.40723300	0.00000000

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CO\_Au<sub>20</sub>  
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79	-1.13529700	3.32345800	-3.72272500
79	-0.43227900	2.29902100	4.55547600
79	-1.48400400	0.10430900	3.11544800
79	-2.36144600	-1.96073600	1.55547600
79	1.52895000	1.01453900	2.97160600
79	-0.73502200	2.86733800	1.80275000
79	-1.82540100	0.62673700	0.23936400
79	0.51735600	-1.30290300	1.45732500
79	-3.12388500	-4.01925800	-0.22325400
79	1.29257700	1.57805100	0.08756200
79	3.26836100	-0.25648200	1.28484300
79	-0.36337500	-3.42964900	-0.38299400
79	-2.63665900	-1.57225500	-1.56090600
79	-0.96476400	3.20043600	-0.90268600
79	0.22100400	-0.90437100	-1.78626700
79	2.24905100	-2.63853500	-0.51149600
79	-1.97652500	0.82505800	-2.70121900
79	2.99051900	0.11500400	-1.82816900
79	1.03375200	1.72974400	-2.84651300
79	4.88212800	-1.59491000	-0.61032000
6	-5.32684700	-0.52800500	-0.39159600
8	-5.33713800	0.35063300	0.35984800

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CO\_Au<sub>2</sub>  
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79	-0.00003700	-1.59832500	-0.00000000
79	-0.00000000	0.95745400	0.00000000
6	0.00005600	2.95798200	0.00000000
8	0.00031900	4.11011500	0.00000000

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CO\_Au<sub>3</sub>  
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79	0.00000000	1.30645500	-0.00000000
79	1.41806600	-1.00264700	0.00000000
79	-1.41846000	-1.00200700	0.00000000

6	0.00164000	3.27978000	-0.00000000
8	0.00266300	4.43487600	-0.00000000

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CO\_Au<sub>4</sub>  
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79	0.00016800	1.24213200	0.00003100
79	2.45116800	-0.24530300	0.00003700
79	-2.45132900	-0.24457100	0.00003700
79	-0.00028800	-1.43978700	-0.00007500
6	0.00111900	3.22007600	-0.00007800
8	0.00194000	4.37429300	-0.00024500

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CO\_Au<sub>5</sub>  
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79	0.00143700	-1.09918300	-0.07768000
79	-1.39336900	1.45730200	-0.12644100
79	-2.71831700	-0.96787000	-0.09339800
79	2.72052800	-0.96282300	-0.01698900
79	1.41052700	1.46000200	-0.23525600
6	-0.54033200	1.09077000	2.87723900
8	0.19979000	0.29356200	3.27099000

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CO\_Au<sub>6</sub>  
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79	1.56504000	0.65595800	-0.11635000
79	0.38765400	3.10856000	-0.08684300
79	-2.89481400	-1.22183400	-0.09545700
79	-0.21117000	-1.69167100	-0.04578500
79	2.50633600	-1.89472100	-0.09617900
79	-1.35618000	1.02052300	-0.11714400
6	-0.06109500	-0.49458700	2.94841900
8	0.07677300	0.59989600	3.29654900

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CO\_Au<sub>7</sub>  
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79	-1.12286100	0.76241100	-0.01123600
79	0.15020000	3.17382600	-0.11469500
79	-3.77339400	-0.13930900	0.00894600
79	3.61480500	-1.00314300	-0.06080700
79	0.99268500	-1.78198600	-0.12783300
79	1.77446500	1.01154200	-0.11236200
79	-1.73751200	-2.00006700	-0.13830300
6	0.01758400	-0.02413100	2.79821200
8	0.99023500	-0.21173500	3.39470000

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CO\_Au<sub>8</sub>  
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79	1.85041900	0.92145800	-0.05850100
79	-0.91808300	1.84954300	-0.04944700
79	1.19238600	3.54938000	-0.07636600
79	-3.54854900	1.19771500	-0.08055500
79	-1.85321900	-0.91505400	-0.05794200
79	0.91607600	-1.84687900	-0.07126900
79	3.54524800	-1.19262100	-0.08790300
79	-1.19549100	-3.54390500	-0.08256900
6	0.02688600	-0.03445300	2.53067700
8	0.09057700	-0.16807400	3.67695700

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CO\_Au<sub>9</sub>  
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79	-1.41989400	-0.00203600	1.08030300
79	-2.25370000	2.40269100	-0.22503900
79	2.47149900	0.00116000	-0.13573200
79	0.46043900	-2.11490200	-0.14931700
79	-3.75569700	-0.00112100	-0.47067600

79	-2.25064400	-2.40397000	-0.22940500
79	3.13014200	-2.62623900	-0.14575400
79	0.45753000	2.11474500	-0.14999300
79	3.12675200	2.62925700	-0.14901200
6	-0.26732100	0.00053400	2.76735700
8	0.53203100	0.00368400	3.59890400

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CO  
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6	0.00000000	0.00000000	-0.66157700
8	0.00000000	0.00000000	0.49618300

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H<sub>2</sub>O\_Au<sub>10</sub>  
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79	-4.29447100	-0.00005300	-0.02450100
79	1.47231900	-0.00007100	0.16256800
79	2.83148400	-2.44850300	-0.06316700
79	-1.46486600	0.00008900	-0.06921400
79	-0.00318800	2.44027600	-0.09174100
79	4.25768900	0.00008200	-0.07119000
79	2.83156700	2.44848100	-0.06278800
79	-2.83407600	2.42986100	-0.01804600
79	-0.00326500	-2.44035700	-0.09168300
79	-2.83382800	-2.42983100	-0.01769900
8	0.43186400	0.00011300	2.75128400
1	-0.12295400	-0.80341800	2.71967900
1	-0.12166200	0.80452300	2.71951100

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H<sub>2</sub>O\_Au<sub>11</sub>  
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79	3.74432300	-1.72675300	-0.00965300
79	-1.12039000	-2.67162900	-0.08316900
79	1.54199200	-3.61178500	-0.27496900
79	-2.19368900	2.82535300	0.01272600
79	2.75893900	3.63429700	-0.16229500
79	-4.35066000	0.99709800	-0.10949100
79	0.49831800	2.03075100	-0.09211200
79	-1.58578900	0.11974900	0.04307600
79	3.25624000	0.96789100	-0.13745500
79	-3.77354600	-1.71603800	-0.00125300
79	1.06953900	-0.90970000	0.46598700
8	1.22318800	0.36978800	2.74661100
1	2.02202600	0.93165200	2.72732400
1	0.41551300	0.91066800	2.83985100

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H<sub>2</sub>O\_Au<sub>12</sub>  
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79	0.12301400	1.10219200	1.51094200
79	-0.10570500	0.85434400	-1.51134100
79	1.65583500	3.07471700	0.19968400
79	0.93862700	-1.45146300	2.14847400
79	1.38714800	-1.53239400	-1.33676200
79	2.83641400	0.63010700	0.08450400
79	4.14669100	-1.61029800	-0.75912000
79	-3.88408400	-1.82971900	-0.06796100
79	-2.97963300	0.76951200	-0.39421500
79	-1.33361800	-1.68895400	-1.40110300
79	-1.50776200	3.03301200	-0.33809000
79	-1.66339600	-1.03340400	1.57761200
8	2.94797100	-2.49448000	2.27375200
1	3.49053900	-2.35528900	1.46281500
1	3.45677700	-2.78347700	3.04987500

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H<sub>2</sub>O\_Au<sub>13</sub>  
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79	-1.61917100	3.38913800	-0.16993300
79	-1.36977600	-1.28967100	-1.60968700
79	1.39842300	-1.26335100	-1.60691900
79	-0.01088600	1.21686300	-1.46351100
79	2.74333000	0.97865500	-0.00137500
79	1.55071400	3.41842000	-0.17164200
79	3.79622100	-1.56795400	-0.00566600
79	-1.34994200	-1.26345200	1.52824300
79	-0.01075100	1.55932600	1.45137800
79	1.37270200	-1.23619400	1.53633100
79	-3.76609500	-1.63886000	-0.00797600
79	0.03642600	-3.35937100	0.03408300
79	-2.76358600	0.92806100	-0.00464700
8	-0.03453900	1.06333500	3.79037400
1	-0.28465200	1.54680000	4.59861000
1	-0.04002700	0.08936400	3.89275600

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H<sub>2</sub>O\_Au<sub>14</sub>  
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79	-2.77328200	2.82339300	0.03522700
79	-2.00356700	-2.07555400	0.04250100
79	-1.40266400	0.85036500	-1.59639900
79	-1.39459500	0.67288800	1.45130100
79	-0.00418400	-1.47344800	2.43056600
79	-0.01113700	-1.47707000	-2.09451900
79	0.01650800	3.05016000	0.09255200
79	-0.02212800	-4.00193300	-0.58572300
79	1.40413800	0.65969500	1.45361200
79	1.41185000	0.83110200	-1.59426400
79	1.97973800	-2.09557600	0.03986300
79	2.80336700	2.79292900	0.03455100
79	3.81282300	-0.05673800	-0.04147200
79	-3.81225100	-0.01543700	-0.03842900
8	-0.02814700	-3.72426500	2.92491200
1	-0.02803000	-4.28474100	2.12282100
1	-0.11150800	-4.21860500	3.75781400

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H<sub>2</sub>O\_Au<sub>15</sub>  
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79	2.88688500	2.29618400	-0.07095500
79	-0.03417000	-1.17897200	-1.51271900
79	3.20057800	-0.38403800	1.02353800
79	0.27700500	1.63540000	-1.57566700
79	-0.39104100	-3.60399000	-0.15034000
79	0.68094100	-1.48981300	2.20621300
79	-2.27503600	0.49593800	-1.85795000
79	0.68365600	1.15649100	1.53120900
79	0.44114300	3.81085300	0.37601400
79	-2.72763300	-2.08301000	-0.42605900
79	-2.01773000	2.41870900	0.39305000
79	-1.71711800	-0.26268200	1.67411200
79	-4.14370100	0.41272600	0.41118000
79	2.60879800	-0.04562900	-1.83726300
79	2.32439900	-2.71235800	-0.53508400
8	1.53640100	-3.59916200	2.75428000
1	1.68083400	-3.99799300	3.63008700
1	2.06683500	-4.00768600	2.04270100

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H<sub>2</sub>O\_Au<sub>16</sub>  
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79	2.65793700	1.59269900	1.87015300
79	0.62348700	2.55969300	0.15255500
79	-3.91933000	-1.01002500	-1.01970700
79	-1.13786300	-1.30138900	-1.39255000
79	-2.35599000	-3.46618400	0.19478400

79	0.28243100	-2.77545900	0.89248800
79	1.61998100	-1.35422900	-1.54418500
79	-2.45393900	1.33613400	-0.99391100
79	-2.28061700	-0.95010500	1.50953700
79	0.17241200	0.82865300	-2.52095100
79	0.34705200	-0.12521400	2.19661800
79	4.38479900	-1.18492200	-1.14004200
79	2.72527700	-1.35307200	1.29578000
79	2.89276500	1.18675600	-0.88925500
79	-1.78067500	1.69322600	1.93815900
79	-1.78605000	3.92308100	-0.14691000
8	0.04592800	3.06070100	-3.21163800
1	-0.53166300	3.57117400	-2.60507500
1	0.82164000	3.57146100	-3.50429000

H<sub>2</sub>O\_Au<sub>17</sub>

79	-0.91934300	-3.69829700	-0.48001400
79	-1.31661100	3.62156300	0.43600700
79	0.66803000	2.38251700	-1.26680200
79	0.72436600	1.90054400	1.70719900
79	3.11044300	1.90461700	0.14265600
79	-2.13057200	1.53729200	-1.32465200
79	-2.02512500	1.09796900	1.69993300
79	2.52398900	0.43032500	-2.29829300
79	2.62913300	-0.19039100	2.14776100
79	-0.30432000	0.43488400	-3.26690300
79	-0.28643300	-0.35154900	3.31255300
79	3.27733200	-1.54584600	-0.33768200
79	-4.03661700	-0.17958500	-0.00957300
79	-1.98399900	-1.30530900	-1.72799700
79	-1.89069500	-1.69095700	1.29338900
79	0.87723200	-1.87249400	-1.85730500
79	0.96410200	-2.26298700	1.19066600
8	0.88945700	-1.59397400	5.00385000
1	1.75636800	-1.92028600	4.69749100
1	0.53599000	-2.09932600	5.75734000

H<sub>2</sub>O\_Au<sub>18</sub>

79	-2.79777100	2.03492700	-1.37914900
79	-1.87085600	-2.00196300	1.23761300
79	0.78428500	-1.34846300	2.36503000
79	-3.42322100	-0.66952800	-0.96649100
79	1.68059800	2.41194600	0.04289900
79	2.80559800	0.56030000	2.07224200
79	-0.04843100	2.55143500	-2.31894900
79	-0.98970600	-0.16103900	-2.56563400
79	0.52262500	-3.36536800	0.40408500
79	-1.71436100	-2.83661500	-1.49419900
79	2.71866700	-1.55285800	-0.18890700
79	1.78721600	0.40779900	-2.16359900
79	4.07943600	0.99400200	-0.63125400
79	1.02038800	-2.31408900	-2.37700500
79	-2.54460000	1.06658400	1.26097700
79	0.16726200	1.52467600	2.42478100
79	-0.92588500	3.36547800	0.50071200
79	-1.78123100	-0.35529800	3.54823400
8	4.17555000	-2.38397200	1.73370400
1	4.91136000	-3.02431700	1.71994300
1	3.55335700	-2.54602900	2.47097200

H<sub>2</sub>O\_Au<sub>19</sub>

79	1.18787100	2.69683500	-1.55923600
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79	-4.34926900	2.10383800	-1.45155200
79	4.01097500	2.69642000	-1.44065700
79	-0.13541700	1.87962300	0.90777400
79	-3.08160000	1.51080300	1.00782900
79	-0.00237500	0.02875200	-1.75746100
79	-2.94770500	-0.35396600	-1.52126900
79	2.83159100	1.93186800	1.01688200
79	2.97279800	0.06532400	-1.51107200
79	-1.57458000	0.79954900	3.23252300
79	-1.57983400	-1.04860500	0.96064500
79	1.43258600	1.01294900	3.23636800
79	1.71309100	-0.81713300	0.96844700
79	-1.40485700	-2.60999100	-1.48701700
79	1.76673000	-2.38607800	-1.47933100
79	0.11392500	-1.68312400	3.27850400
79	0.23816100	-3.39036800	1.08181600
79	0.34449300	-4.82011800	-1.38306000
79	-1.55395200	2.50414100	-1.56131100
8	0.12288300	-0.84568900	-4.23847400
1	0.99353600	-1.28131000	-4.32163600
1	-0.60470700	-1.49009500	-4.33758700

H<sub>2</sub>O\_Au<sub>1</sub>

79	-0.28968300	0.00000000	0.00023000
8	2.18172100	0.00000600	-0.01279400
1	2.71552700	-0.81142700	0.04208400
1	2.71565300	0.81135500	0.04208900

H<sub>2</sub>O\_Au<sub>20</sub>

79	1.14878500	4.81557300	-1.31998800
79	-5.11346100	-0.41728100	0.55471200
79	-3.00264600	-1.50059600	-0.98972600
79	-0.83148000	-2.42451000	-2.36943500
79	-2.74190100	-0.73072200	2.05328900
79	-3.15206200	1.51517200	-0.11244900
79	-0.89616100	0.45156200	-1.69527800
79	-0.49456500	-1.86944000	0.50794800
79	1.55774200	-3.21968000	-3.65844200
79	-0.64128900	1.24728100	1.40861300
79	-0.33758400	-0.98227600	3.32541400
79	1.93601200	-2.73290100	-0.89626500
79	1.53127200	-0.45338300	-3.07306800
79	-1.11579000	3.23246200	-0.72299700
79	2.05582900	0.19409800	-0.26406300
79	2.15516500	-2.06240200	1.73681800
79	1.39628900	2.17894000	-2.31326500
79	2.01637800	0.99136300	2.61583900
79	1.65684200	2.95522400	0.75291900
79	2.28190800	-1.17218700	4.41424000
8	4.63992200	-0.07712800	0.26280300
1	4.76112500	-1.04285500	0.34956500
1	4.78607200	0.37236400	1.11746200

H<sub>2</sub>O\_Au<sub>2</sub>

79	-1.50174800	-0.00008500	-0.00000500
79	1.06458100	0.00018500	0.00000800
8	3.34726200	-0.00058400	0.00005100
1	3.87745700	-0.81457000	-0.00033800
1	3.88062300	0.81132100	-0.00033900

H<sub>2</sub>O\_Au<sub>3</sub>



79	-1.39849500	0.09641700	0.00002500
79	1.02389300	-1.45918700	-0.00002400
79	0.82296300	1.48003900	0.00000400
8	-3.44771900	-0.87756400	0.00020600
1	-4.29314400	-0.39959500	-0.00388800
1	-3.54556500	-1.84418800	0.00187400

H<sub>2</sub>O\_Au<sub>4</sub>

79	-0.00049100	1.28592200	-0.00011700
79	-2.46963500	-0.18017100	0.00014400
79	2.46969400	-0.18033200	0.00014200
79	0.00010800	-1.38960400	-0.00016200
8	0.00257100	3.56100700	-0.00013100
1	-0.81105900	4.09124600	0.00003300
1	0.81611600	4.09137100	0.00044500

H<sub>2</sub>O\_Au<sub>5</sub>

79	0.00012900	0.97582400	-0.00004100
79	1.38314700	-1.53794800	-0.00003300
79	2.81087900	0.82941700	0.00007300
79	-2.81060800	0.82974900	0.00006700
79	-1.38358400	-1.53779100	-0.00002200
8	0.00026100	3.37527900	-0.00026800
1	0.81467800	3.90813000	-0.00088300
1	-0.81376800	3.90872200	-0.00049400

H<sub>2</sub>O\_Au<sub>6</sub>

79	-0.91976500	1.44478800	-0.00038600
79	-3.23707900	0.00154700	-0.00044800
79	1.43798900	-2.76961800	0.00009700
79	1.66203100	-0.00039000	-0.00006900
79	1.44042600	2.76865800	0.00070900
79	-0.92127200	-1.44458400	0.00062400
8	4.13995400	-0.00315300	-0.00351900
1	4.67822600	0.80740600	-0.01825600
1	4.67818900	-0.81382400	0.00477400

H<sub>2</sub>O\_Au<sub>7</sub>

79	-1.12070100	0.81515000	0.17031100
79	0.20587500	3.18449400	-0.21116900
79	-3.75491500	-0.16319500	0.10252200
79	3.61232700	-1.02060300	0.14121900
79	1.01471900	-1.81259800	-0.17184900
79	1.78122600	1.00168700	-0.07615600
79	-1.71445600	-1.96857600	-0.28020700
8	-0.26309800	-0.20410800	2.57737900
1	0.70713300	-0.09396300	2.60259300
1	-0.50424500	-1.14558500	2.47934500

H<sub>2</sub>O\_Au<sub>8</sub>

79	2.10828000	0.11738200	-0.07216300
79	-0.11935900	2.00811600	-0.04562200
79	2.32872000	2.65772800	-0.99679700
79	-2.60753400	2.32978000	0.98219100
79	-2.14600800	-0.12000900	-0.10994300
79	0.06859700	-1.98251300	0.12501800
79	2.67449400	-2.34333400	0.87843500
79	-2.28936300	-2.63047600	-1.08287200
8	-0.18262000	-0.39153400	2.55104000
1	0.77101900	-0.18256400	2.58930200

1 -0.71838200 0.41750500 2.42082200

H<sub>2</sub>O\_Au<sub>9</sub>

79 1.21220600 -0.00192800 0.73975400  
79 2.28387100 -2.45545800 -0.08302800  
79 -2.36090400 0.00125300 -0.15655200  
79 -0.44399600 2.26295300 -0.08466600  
79 3.83285100 -0.00057200 -0.38075400  
79 2.28645800 2.45444000 -0.07029800  
79 -3.14459300 2.59868700 -0.11033200  
79 -0.44649800 -2.26365900 -0.08707300  
79 -3.14787900 -2.59505300 -0.09747100  
8 -0.45471300 -0.00535400 2.60719300  
1 -1.00700700 -0.81144300 2.61928300  
1 -1.00496900 0.80192700 2.62641800

H<sub>2</sub>O

8 0.00000000 0.00000000 0.10951200  
1 -0.00000000 0.80334700 -0.43804900  
1 -0.00000000 -0.80334700 -0.43804900

NO<sub>2</sub>\_Au<sub>10</sub>

79 1.60652600 -1.54998000 -1.09610900  
79 -0.53690000 0.36823500 -1.06654400  
79 -3.55379300 -1.03829300 -0.34229200  
79 2.01106100 -0.44581000 1.63169300  
79 2.07309100 1.66485400 -0.47241000  
79 -2.77091900 1.70203100 0.23707600  
79 -0.31752600 3.02690500 -0.35253100  
79 4.02994000 -0.36911100 -0.19250300  
79 -1.72154200 -0.80540100 1.59821100  
79 -0.98206900 -2.35565600 -1.05086500  
7 0.81819300 -0.63652000 3.41882800  
8 -0.48676900 -0.78641400 3.40053400  
8 1.37187900 -0.60965000 4.53245700

NO<sub>2</sub>\_Au<sub>11</sub>

79 -3.55435600 -1.97839600 -0.83807700  
79 1.10435800 -2.64543700 -0.17203300  
79 -0.84536500 -0.92083500 -1.31711100  
79 2.11958800 2.73913900 -0.63181200  
79 -2.86787700 3.18431400 0.62724200  
79 4.15447600 1.00841900 0.38888400  
79 -0.53151900 1.89878900 -0.10967600  
79 1.62317400 0.04615400 -0.43625400  
79 -3.12307300 0.57230300 0.11628600  
79 3.76684400 -1.73633400 0.27239400  
79 -1.86664400 -1.85206700 1.30431500  
7 0.42416400 -1.07345400 3.06567600  
8 0.30315200 -0.14047300 2.21956800  
8 -0.47288600 -2.04123200 2.95690900

NO<sub>2</sub>\_Au<sub>12</sub>

79 -0.09363400 1.38364800 1.52193900  
79 -0.08900900 0.96202700 -1.46122300  
79 1.60127800 3.07350300 -0.51791200  
79 1.71202400 -1.23332200 1.58277900  
79 1.01682300 -1.68203500 -1.19276900  
79 2.81757700 0.68127400 -0.45937500  
79 3.70176400 -1.95367500 -0.29573000

79	-3.76927100	-1.95143900	0.18271200
79	-2.79743200	0.59908000	0.29594200
79	-1.63327200	-1.32151000	-1.86868900
79	-1.71530800	3.06645800	-0.03898100
79	-1.09521200	-1.70219700	1.11366100
7	1.21465400	0.31537300	4.36946500
8	1.72484300	-0.69536800	3.76092600
8	0.60609900	1.19150900	3.65003800

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NO<sub>2</sub>\_Au<sub>13</sub>  
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79	0.87028500	3.83849000	-0.15404200
79	1.38070300	-1.23738400	1.66003100
79	-0.98115600	-2.40462900	0.29191200
79	-0.59855300	1.75216900	1.68359600
79	-2.61382200	0.04623000	0.32136300
79	-2.61803600	2.80820200	0.26077200
79	-3.69594500	-2.44144400	0.45066500
79	1.33202200	-0.86689700	-1.38999300
79	-0.29147400	1.60962300	-1.36426000
79	-1.21056400	-0.74418500	-2.44775400
79	3.85472300	-0.71724600	-0.21620200
79	1.55129500	-3.48773700	0.18110700
79	2.45278100	1.61648800	-0.21827500
7	1.95260400	1.23932200	3.45543500
8	0.91511400	0.61035800	2.81106600
8	2.98279500	0.55990400	3.45859300

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NO<sub>2</sub>\_Au<sub>14</sub>  
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79	0.23735000	3.88769900	-0.25940100
79	3.86869600	-0.28843900	-0.48427000
79	0.23957600	1.84458700	1.83083700
79	-0.23582100	1.54709300	-1.98137000
79	1.17715300	-0.77464600	-1.45022300
79	1.69554200	-0.87746200	1.47102900
79	-2.10517800	2.20034300	0.28947200
79	2.52091500	-3.03966300	-0.20241500
79	-1.62443800	-0.79520600	-1.67460800
79	-1.44189200	-0.45176400	1.37231500
79	-0.24099600	-2.91686400	0.22026400
79	-3.94485400	0.15343900	-0.03259400
79	-3.00927300	-2.63782800	0.20251000
79	2.31219700	1.95162000	-0.41983100
7	2.05311900	0.71122000	4.27926200
8	1.57042600	1.72898000	3.66110700
8	2.07445100	-0.40502900	3.63758300

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NO<sub>2</sub>\_Au<sub>15</sub>  
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79	-3.05549600	-2.77761600	0.34797100
79	-1.30853500	1.47235200	-1.45221000
79	-0.76401500	-1.39161900	1.53294700
79	-1.30774700	-1.47154400	-1.45540600
79	-0.04137000	3.74078800	-0.08505700
79	-0.76089100	1.38897100	1.53446400
79	0.45010300	0.00279500	-2.97740400
79	1.25510500	-0.00385700	2.74960500
79	-0.04131100	-3.74036900	-0.08837400
79	1.63509200	1.60077600	-0.39547600
79	1.63249500	-1.59728100	-0.39648400
79	3.87898600	-0.00163400	0.82346500
79	3.50929400	0.00084900	-1.83722900
79	-3.29203700	0.00059500	0.35485600
79	-3.05365700	2.77849100	0.35264300

7	4.30345300	-0.00502600	2.95203900
8	3.27121600	-0.00649000	3.76477300
8	5.44511100	-0.00588300	3.44512800

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NO<sub>2</sub>\_Au<sub>16</sub>  
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79	2.05539200	-0.26571300	2.47225000
79	2.41116500	2.51786500	1.34224600
79	-4.38272100	0.56647400	-1.16323200
79	-1.76980200	-0.07061800	-2.06184500
79	-2.37871600	-3.43343300	1.24509400
79	-0.77800600	-2.42464200	-0.86743200
79	0.88017700	-0.74643900	-2.22240800
79	-2.40193900	2.16656700	-0.11800200
79	-2.66622900	-0.65078700	0.86495500
79	0.57756200	2.27456900	-1.12942300
79	-0.20169400	-1.83022500	2.10629100
79	3.69387400	-1.75718600	-1.82606000
79	2.05382800	-2.20819200	0.35224900
79	3.14838000	0.49687800	-0.32938100
79	-0.27228300	1.00344000	1.43756400
79	-0.47216100	3.85587500	0.94053200
7	1.89172400	1.88446400	-4.00339200
8	1.14436100	2.62605500	-3.24788000
8	2.16922500	0.71751600	-3.55269300

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NO<sub>2</sub>\_Au<sub>17</sub>  
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79	1.45054500	-2.16780300	-2.42237600
79	-2.92019900	1.24090800	1.97300000
79	-0.75348600	2.17692100	0.21267400
79	-0.18208900	0.54272600	2.56106100
79	1.38953100	2.73907700	2.10723000
79	-2.89221200	0.26492400	-0.76837300
79	-1.97519800	-1.46728900	1.46726100
79	1.03940800	3.00249400	-2.09073100
79	2.77438800	0.00709000	1.93211200
79	-2.02051800	2.32211000	-2.37491700
79	0.38628900	-2.18077900	2.95670600
79	2.46421600	1.25944800	-0.55702500
79	-3.74121000	-2.43699300	-0.52381200
79	-1.20138800	-2.11136700	-1.64226100
79	0.89054500	-1.41872100	0.26993100
79	0.14501600	0.31161800	-2.16528200
79	3.83335300	-1.24033200	-0.26892700
7	4.43636700	-2.61833100	-1.92612600
8	3.50622200	-2.96312900	-2.80133000
8	5.57791400	-3.08066500	-2.09273200

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NO<sub>2</sub>\_Au<sub>18</sub>  
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79	-3.54011500	-2.27950400	-1.14426200
79	-0.77575400	1.53753300	-0.70904700
79	3.06273100	0.96599400	-1.86563000
79	-3.48062000	0.39688200	-0.18452600
79	1.16163100	-2.68751900	0.88753200
79	3.63320300	-1.21535000	-0.34643200
79	-1.57595400	-1.56964100	0.97959700
79	-2.10174100	0.70016100	2.61568300
79	1.56597800	3.23265400	-0.24601500
79	-2.81100900	2.92384400	0.91871100
79	1.98410400	0.71923800	0.99641200
79	0.26116700	-0.62594800	3.00692800
79	2.99736700	-1.47283000	2.65515400
79	-0.01273600	2.56458600	1.91900700

79	-1.62789900	-0.66117500	-2.40448800
79	1.08471500	-1.13326200	-1.65537000
79	-0.68408300	-3.39044800	-1.05901600
79	0.24408500	1.06316000	-3.35889900
7	2.17846400	3.64674400	-3.61869800
8	2.72578900	3.19056300	-2.51438200
8	1.44049800	2.81834000	-4.24695600

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NO<sub>2</sub>\_Au<sub>19</sub>  
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79	2.97273000	-0.48344400	-1.30492100
79	1.00873500	4.75962500	-1.55122000
79	3.60386100	-3.24207700	-1.29067900
79	1.84895300	0.63802100	1.04520000
79	0.65144400	3.51746100	0.91747300
79	-0.03067200	0.01581800	-1.72725600
79	-0.98220600	2.75933700	-1.58019200
79	2.56849300	-2.33821700	1.06078000
79	0.63030500	-2.85321400	-1.42930600
79	0.35269800	1.94783800	3.13278400
79	-1.31985000	1.22536500	0.88554000
79	1.33481000	-1.16380000	3.29328500
79	-0.37879500	-1.97428500	0.98870400
79	-2.85318500	0.74303300	-1.53936200
79	-2.07642400	-2.29994600	-1.23794500
79	-1.71247700	-0.56307000	3.15776000
79	-3.40471600	-0.92613100	1.04926400
79	-4.74456900	-1.35162200	-1.38531800
79	2.15796500	2.13825300	-1.35359100
7	1.39580000	-1.89409300	-4.34594600
8	1.21906200	-2.97749200	-3.66663400
8	1.24201100	-0.78601700	-3.69929600

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NO<sub>2</sub>\_Au<sub>1</sub>  
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7	2.29188100	0.03249400	-0.00020900
8	1.54253600	1.08292800	0.00012400
8	1.64188500	-1.07024800	0.00012000
79	-0.52555100	-0.00416300	-0.00000600

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NO<sub>2</sub>\_Au<sub>20</sub>  
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79	2.01950400	1.95785900	-4.28318700
79	0.61909900	-5.12030300	0.02480700
79	1.22853800	-2.83189100	1.58216800
79	1.73438200	-0.47679800	2.88376800
79	-1.45802600	-3.21414400	0.01331600
79	1.23287800	-2.84767200	-1.55295300
79	2.38933100	-0.67444300	0.00571700
79	-0.85058000	-0.76778000	1.55958300
79	2.00902500	1.99866500	4.26903900
79	-0.84491900	-0.78207700	-1.55255500
79	-3.31552700	-1.20608500	0.00054300
79	-0.45906300	1.84754900	2.88595600
79	2.11586900	2.32153800	1.50564100
79	1.74193700	-0.50484100	-2.87553000
79	-0.40412900	2.03961300	-0.00984000
79	-2.82740700	1.44079800	1.57790600
79	2.12029700	2.30574600	-1.52216000
79	-2.82274300	1.42679000	-1.59807700
79	-0.45067500	1.82079600	-2.90347900
79	-5.12135600	0.96915500	-0.01140900
7	4.28646600	0.68681500	0.00333100
8	4.04637600	2.00716300	-0.00587600
8	5.47067800	0.32995300	0.01032400

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 NO<sub>2</sub>\_Au<sub>2</sub>  
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79	-1.37717700	-0.27090200	-0.00013600
79	1.32017000	-0.36843100	0.00013700
7	0.21726200	2.65301400	-0.00007200
8	-0.91495000	2.05484200	0.00167600
8	1.28778700	1.93718200	-0.00162200

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 NO<sub>2</sub>\_Au<sub>3</sub>  
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79	-0.75001100	-1.25288400	-0.00001900
79	1.82625500	-0.32246400	0.00001600
79	-0.19154600	1.52048200	-0.00000900
7	-2.70644300	-0.12555200	0.00001300
8	-3.88097000	-0.52785100	0.00010100
8	-2.48727700	1.17951700	0.00000700

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 NO<sub>2</sub>\_Au<sub>4</sub>  
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79	0.31561700	-1.55263100	-0.00015900
79	-2.28236800	-0.67197700	0.00009600
79	2.50353700	0.13561600	0.00008300
79	0.12363500	1.36991700	0.00002800
7	-1.83279400	2.32350600	-0.00020800
8	-2.88115100	1.51961000	0.00042400
8	-2.03681600	3.54819400	-0.00070900

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 NO<sub>2</sub>\_Au<sub>5</sub>  
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79	-0.09455600	-1.15012200	0.01609800
79	-1.60861400	1.33461400	-0.03616800
79	-2.85498000	-1.00586200	0.02099200
79	2.64107600	-1.36979300	0.00999100
79	1.71105200	1.13229900	-0.04307800
7	0.37344400	4.01743200	0.14748600
8	1.57655600	4.24673700	0.29521600
8	0.13114900	2.69428600	-0.10664000

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 NO<sub>2</sub>\_Au<sub>6</sub>  
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79	-2.50739500	0.07806300	-0.00089400
79	-1.84791600	-2.49033300	0.00415300
79	3.00594500	-1.35664700	-0.00669900
79	2.27311100	1.30946700	0.00566600
79	-0.18157400	2.41899200	0.00102500
79	0.26406800	-0.72514000	-0.00009700
7	-3.45291000	3.13659500	-0.01256600
8	-2.38485600	2.27816800	-0.00083000
8	-4.53045300	2.53759200	-0.01930800

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 NO<sub>2</sub>\_Au<sub>7</sub>  
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79	1.38932000	1.06418300	0.00030000
79	-0.13939500	3.30104100	0.00040500
79	3.87990200	-0.07899000	-0.00068000
79	-3.89645300	-0.39349700	0.00003500
79	-1.73310200	-1.89838200	-0.00106400
79	-1.51587700	0.97608400	0.00018000
79	1.85281600	-1.77670200	0.00001200
7	0.18636300	-4.44569900	0.00311500
8	1.35654000	-4.82565700	0.00560900
8	0.08792400	-3.07252200	-0.00030600

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 NO<sub>2</sub>\_Au<sub>8</sub>  
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79	2.25008600	0.63317700	-0.00060600
79	0.11006000	-1.60046700	-0.00045200
79	2.76022200	-2.18130700	0.00184300
79	-2.16111500	-3.13742000	-0.00155100
79	-2.57686400	-0.44202500	0.00001500
79	-0.41446500	1.49910800	0.00031700
79	1.66766100	3.28034800	-0.00143500
79	-3.08552900	2.19050800	0.00171800
7	5.44363200	-0.74876600	0.00040300
8	4.60709800	0.21541200	-0.00210300
8	4.94790300	-1.94922500	0.00324200

NO<sub>2</sub>\_Au<sub>9</sub>

79	-0.91885900	-0.43456500	-0.61388600
79	-0.37370500	-2.98432800	0.04278500
79	2.88530300	1.00641100	0.97857200
79	-0.31616200	2.22418600	0.45564400
79	-3.09457400	-1.71890700	0.97477300
79	-3.23879700	0.90013500	0.34139200
79	-1.58482300	1.99306900	-1.87973900
79	1.75812500	-1.28770500	-0.43142200
79	4.35906300	-0.47990000	-0.65087400
7	2.01625000	2.39204700	2.39807700
8	2.63161700	2.78882100	3.39963200
8	0.78290200	2.83648300	2.23175200

NO<sub>2</sub>

7	-0.00000000	0.00000000	0.33093100
8	0.00000000	1.13574800	-0.14478200
8	-0.00000000	-1.13574800	-0.14478200

NO\_Au<sub>10</sub>

79	-4.27574500	-0.00021200	-0.01004100
79	1.44951700	-0.00032500	-0.08576900
79	2.83129000	2.43962900	-0.05843000
79	-1.46058000	-0.00018200	-0.06586800
79	-0.00731100	-2.43579200	-0.09523700
79	4.26209700	-0.00017600	-0.02592900
79	2.83145700	-2.44010000	-0.05820900
79	-2.84370000	-2.43857700	-0.04187900
79	-0.00732200	2.43538000	-0.09660700
79	-2.84363400	2.43823100	-0.04301300
7	0.95611100	0.01072400	2.93859500
8	-0.20529300	0.01159700	3.16592200

NO\_Au<sub>11</sub>

79	-0.01301000	1.41556400	2.27759700
79	-2.57060200	0.14698700	-1.06342500
79	-2.27377200	2.51572100	-2.35067700
79	0.93104500	-3.17755800	-0.82754900
79	4.65699500	0.76368000	-0.31426800
79	0.10335600	-0.83934400	0.33913500
79	2.85459500	-1.25703900	-0.57628000
79	-2.62347800	-0.64609400	1.81951300
79	2.14878400	1.33464400	0.61725400
79	-2.37352500	-2.44472400	-0.24788500
79	-0.43816500	2.04050800	-0.39576500
7	-2.64350200	0.37760000	3.68235800
8	-1.65888300	1.12769400	3.91113800

NO\_Au<sub>12</sub>

79	-0.06314700	1.06788900	1.45085500
79	-0.01797800	0.97803800	-1.58092100
79	1.63078400	2.99107300	-0.25610300
79	1.37756600	-1.33428100	1.55248000
79	1.18619400	-1.58620800	-1.52638100
79	2.86955100	0.60571300	-0.30135900
79	3.65508700	-2.03321500	-0.13703200
79	-3.84484300	-1.85707400	0.14140400
79	-2.92861600	0.74850600	0.11307800
79	-1.54553600	-1.36992300	-1.57679500
79	-1.58835600	3.08593400	0.00437600
79	-1.35510900	-1.45092600	1.50606500
7	3.46640700	0.21639300	3.11274700
8	3.13288100	1.33609200	3.30339400

NO\_Au<sub>13</sub>

79	-0.21135300	1.49433800	2.50580500
79	1.84667000	-2.24709100	-0.98273900
79	1.03076300	0.42670400	-1.97551900
79	-0.82195800	-1.63494400	-1.27019600
79	-3.45187100	-0.42683300	-0.27309800
79	-2.79987400	-2.93850300	0.53549600
79	-3.69839400	2.11951900	-1.15499600
79	3.49889200	0.95035100	-0.80548100
79	-1.21083400	-0.92810900	1.75851600
79	-1.19021300	1.42652500	-0.30444100
79	3.96248800	-1.52788500	0.68058000
79	1.49639700	2.76871200	-0.16610600
79	1.46631900	-0.24951200	1.11783000
7	0.72103800	4.26404800	1.19802500
8	0.18840100	3.84038400	2.25341800

NO\_Au<sub>14</sub>

79	-0.51762200	3.97204000	0.26814100
79	3.67809200	0.46313400	-0.10254700
79	0.15544500	1.48029100	1.55793600
79	-0.46044300	1.81359600	-1.69103100
79	1.29259900	-0.30922900	-1.48898000
79	1.47712100	-0.91811200	1.66443900
79	-2.57034600	1.88223300	0.40399100
79	3.06856700	-2.39687500	-0.49208300
79	-1.48294700	-0.73489000	-1.60560300
79	-1.29425700	-0.87905900	1.43973500
79	0.30600800	-2.95272300	-0.32865000
79	-3.89678100	-0.52314700	0.19166500
79	-2.47672600	-3.08974800	-0.14330600
79	2.07474900	2.68561800	-0.28003500
7	3.38835900	-2.06049500	2.86189100
8	3.41976200	-3.06672500	3.48331200

NO\_Au<sub>15</sub>

79	1.75062100	-3.00560300	0.75029600
79	-1.47950800	-0.49991600	-1.95145800
79	-0.36569000	-1.03801000	1.58350100
79	1.15339100	-1.06180100	-1.49189600
79	-4.26181800	0.12007300	-1.59568800
79	-2.23291700	0.77705900	2.57282500
79	0.29202500	1.64421400	-1.49279300
79	2.48348800	-0.26665100	1.54529100
79	3.81546700	-1.50653200	-0.66224300



79	-2.39928200	1.72506000	-0.23160400
79	3.17305300	1.21976200	-1.01698300
79	-0.14013800	2.30113400	1.33009800
79	1.88433800	3.60458300	-0.27996200
79	-0.96462000	-3.06455700	-0.26062400
79	-3.07669900	-1.24856900	0.60355700
7	2.38655700	1.09239900	3.14708300
8	1.54861000	2.00422300	3.14842200

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NO\_Au<sub>16</sub>  
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79	1.97772900	1.00278800	2.09291200
79	1.62912100	3.16062000	0.04400900
79	-4.08694400	-1.03567900	-0.97930800
79	-1.27835100	-1.13015200	-1.45636200
79	-2.40037500	-2.86435000	0.67732200
79	0.33301300	-3.32787800	0.26546100
79	1.45489400	-1.24841300	-1.80084000
79	-2.78366300	1.42651600	-1.20042300
79	-2.83761600	-0.15630400	1.69502400
79	0.19241000	1.24050400	-1.61313500
79	-0.13869900	-0.90097500	1.79721500
79	4.19764500	-1.61279100	-1.26329400
79	2.54772900	-1.60248100	1.13967300
79	3.12307800	0.89398200	-0.60845300
79	-0.94303800	1.79943600	1.26754400
79	-1.15495300	3.75666600	-0.80976500
7	1.40978000	2.80503900	4.01032600
8	0.42563900	3.45588100	3.92110900

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NO\_Au<sub>17</sub>  
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79	-2.90168900	2.62601900	-0.71217600
79	0.89256200	-3.88624700	0.32996600
79	1.42335600	-1.51834300	1.92140600
79	2.07667800	-1.70868000	-1.12527600
79	3.99260400	-0.39302600	0.41250100
79	-1.19845600	-2.12995200	1.08483300
79	-0.47896200	-2.48114400	-1.93283000
79	1.70179300	1.26482700	1.95636700
79	2.33915800	1.25289800	-1.10420300
79	-0.53302800	0.06322800	3.17661500
79	0.56305100	-0.06549800	-3.11028700
79	1.62535800	3.65430400	0.30615400
79	-3.34551000	-2.02892000	-0.70565300
79	-3.11550300	0.29909300	1.11891500
79	-1.70193400	0.16483700	-1.40254900
79	-0.75288400	2.30121300	1.04035000
79	0.01320600	2.52256100	-1.96582900
7	-2.72623800	0.28124600	3.25334800
8	-3.53754400	0.37435500	4.18132100

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NO\_Au<sub>18</sub>  
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79	-2.40228500	-2.42571600	-1.31478900
79	-2.10791200	1.95095600	0.76607800
79	0.63723200	2.77008200	0.03561600
79	-3.49932600	-0.66122100	0.57500700
79	2.03796500	-1.14618000	-1.65549500
79	2.95475400	1.64358400	-1.16425500
79	0.31942300	-3.39241700	-0.91857300
79	-1.05261200	-2.19124700	1.34997800
79	0.00987600	2.11479700	2.74360200
79	-2.16324600	0.09964200	2.92207100
79	2.20560800	0.79157600	1.57139100

79	1.81234400	-2.14832700	1.16300300
79	4.15041800	-0.85114300	0.25424000
79	0.56478700	-0.83228500	3.36180200
79	-2.28300600	0.33612900	-1.94657400
79	0.48962900	1.23090000	-2.48457600
79	-0.32127400	-1.42399700	-3.17599500
79	-1.65766200	3.10142000	-1.78453400
7	1.75315700	5.20864600	-1.00014500
8	1.48071000	5.64771200	-2.06761700

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NO\_Au<sub>19</sub>  
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79	1.05894600	2.78422900	-1.40486500
79	-4.44482000	1.94739600	-1.39596300
79	3.88517000	2.90717300	-1.39712600
79	-0.21191000	1.83284800	1.00029500
79	-3.17049200	1.34550700	1.04775300
79	-0.00355200	0.03636600	-1.89798500
79	-2.91840400	-0.43695100	-1.44731200
79	2.78199300	2.03008900	1.04715000
79	2.94129500	0.23853900	-1.44984300
79	-1.64245000	0.66615700	3.26472100
79	-1.51662000	-1.14145000	0.97223400
79	1.44861600	1.02117600	3.26481600
79	1.73626700	-0.76576300	0.97123700
79	-1.29014300	-2.63960800	-1.47537400
79	1.85629700	-2.27624500	-1.47793700
79	0.21264400	-1.84071300	3.22947000
79	0.39848600	-3.44279700	0.96870000
79	0.55214600	-4.78719300	-1.50835700
79	-1.66445000	2.47037600	-1.40607200
7	-0.09149600	0.74456000	-5.19600300
8	-0.00902100	-0.14920600	-4.39571200

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NO\_Au<sub>1</sub>  
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7	0.48815400	-1.63996300	-0.00000000
8	-0.42713500	-2.42938000	-0.00000000
79	-0.00000000	0.39132600	0.00000000

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NO\_Au<sub>20</sub>  
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79	-3.15767700	-1.55752400	-3.68324800
79	-0.53499600	5.03953400	0.75405100
79	-0.76632400	2.59994100	2.15641300
79	-0.92169000	0.13215400	3.33200200
79	1.46184600	3.17893700	0.00271500
79	-1.56428700	2.95729500	-0.86178500
79	-1.82061100	0.37836900	0.54421000
79	1.29865700	0.61044900	1.44660700
79	-1.00978800	-2.51237600	4.34036300
79	0.46170900	0.98435300	-1.70230600
79	3.22602900	1.21379500	-0.70097000
79	1.12314400	-2.13083200	2.52708100
79	-1.89778100	-2.35399900	1.66083300
79	-2.41638100	0.79688200	-2.30779600
79	0.28723800	-1.97358700	-0.29283700
79	3.05385100	-1.62474500	0.65623900
79	-2.57667400	-2.05836700	-0.96806200
79	2.24200800	-1.26518500	-2.38066200
79	-0.37995800	-1.45789900	-3.12904600
79	4.88113900	-0.96783600	-1.40059600
7	-4.87199900	0.03009600	0.56845900
8	-5.50786400	0.07874600	-0.43031500

NO\_Au<sub>2</sub>

79	-0.21123300	-1.61203100	-0.00000000
79	0.00000000	0.94463100	0.00000000
7	0.65637000	3.07852500	0.00000000
8	1.51160000	3.89686600	0.00000000

NO\_Au<sub>3</sub>

79	-0.10012900	1.58398000	0.00006900
79	1.18851200	-1.10518600	0.00005300
79	-1.59081200	-0.65195000	-0.00006000
7	2.87081300	0.29067400	0.00000500
8	2.44952900	1.45556900	-0.00061300

NO\_Au<sub>4</sub>

79	0.00426000	-1.48697900	-0.04885000
79	2.44284700	-0.20902100	0.00196500
79	-2.43928500	-0.22481600	0.00277000
79	0.00028600	1.19560200	0.07911900
7	-0.03276900	3.32139000	0.20844800
8	-0.05139600	4.25527200	-0.52805500

NO\_Au<sub>5</sub>

79	-1.57300100	1.21464500	0.06952300
79	2.90495800	-0.71216600	-0.01785800
79	1.27148600	1.43521000	0.03802800
79	-2.47510800	-1.41281600	-0.01961900
79	0.17837600	-1.22423700	-0.02268200
7	-1.70903500	3.30941800	0.27625200
8	-1.53337400	4.01047600	-0.70972200

NO\_Au<sub>6</sub>

79	0.41868700	-1.64759700	-0.12669400
79	3.02197700	-0.86607200	-0.06086100
79	-0.75245100	3.04872300	-0.10049400
79	-1.62886700	0.47162200	-0.09767500
79	-2.24731000	-2.18223300	-0.09828400
79	1.22856300	1.18304700	-0.08668700
7	-0.83077000	-0.13796000	2.90906100
8	0.32601000	0.04674900	3.09017600

NO\_Au<sub>7</sub>

79	0.42183400	1.48344500	-0.52787900
79	-1.90412000	2.74640700	0.03043600
79	2.17030100	-0.00330600	1.42409600
79	-1.96819000	-2.70656000	0.13098900
79	0.37724000	-1.52234100	-0.50887800
79	-2.03162500	0.02238500	0.11677900
79	2.55199600	-0.06458500	-1.40279000
7	2.46825700	-0.04826300	3.50348300
8	1.61809900	0.48221000	4.21477600

NO\_Au<sub>8</sub>

79	1.43517000	-1.48838800	-0.05940100
79	1.50453700	1.42349000	-0.05189900
79	3.64924900	-0.08554500	-0.74102800
79	0.08765500	3.63213100	0.62472400
79	-1.41255300	1.48892800	-0.08103300
79	-1.48366300	-1.42649400	-0.10721700

79	-0.08461800	-3.62425100	0.63486400
79	-3.62587800	0.08640200	-0.77666200
7	0.19048200	-0.25662600	2.74480800
8	-0.85693100	0.16260700	3.10508900

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NO\_Au<sub>9</sub>  
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79	-2.05002500	-1.05253600	1.48974000
79	-3.76513600	0.16733200	-0.11095700
79	1.65056400	-1.30677300	1.48973800
79	1.85671700	1.33238700	0.01965600
79	-0.99231700	1.05620200	-0.34841700
79	0.18859400	3.43876900	0.27043400
79	3.67310500	-0.69528700	-0.30180400
79	-1.58357900	-1.41471600	-1.58660700
79	1.05128500	-1.12938900	-1.49714900
7	0.51528900	-2.13186900	3.05338300
8	-0.73930700	-2.04501500	3.01002100

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NO  
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7	0.00000000	0.00000000	-0.63193600
8	0.00000000	0.00000000	0.55294400

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SO<sub>2</sub>\_Au<sub>10</sub>  
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79	-1.53265900	1.07692900	0.22568500
79	1.45799900	1.05444800	-0.09598300
79	0.14952600	-0.87312100	1.87620000
79	-2.32513600	-1.79319400	0.24329800
79	-0.24595300	-0.62126700	-1.98086800
79	2.45839200	-1.78864600	-0.24757700
79	4.12449700	0.27306100	-0.09872500
79	-0.23151300	2.06768200	-2.17921900
79	0.23860600	1.73179800	2.48002300
79	-4.13986300	0.13042900	-0.05823000
16	0.55711400	-3.43575900	-0.39875300
8	-0.40479300	-2.79672300	0.91876000
8	-0.25416500	-2.75569000	-1.74671600

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SO<sub>2</sub>\_Au<sub>11</sub>  
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79	-3.35435200	-2.45650900	-0.47653500
79	2.21080000	-1.75087900	1.00095300
79	-1.22993600	-1.94772800	1.05730700
79	2.11505000	2.83179100	-0.41656500
79	-2.76689100	2.89146100	0.36730100
79	1.34784900	1.36337400	1.64087000
79	-0.53343400	1.63118700	-0.73482800
79	1.66335800	-0.02680200	-1.29425800
79	-2.95678800	0.23333700	0.07280700
79	4.10514500	-1.37618000	-0.77844100
79	-0.83524700	-1.00300700	-1.83795500
16	0.47340000	-1.14695500	3.90814400
8	0.86427800	0.39492400	3.56989800
8	0.50408000	-1.95268800	2.43233200

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SO<sub>2</sub>\_Au<sub>12</sub>  
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79	1.04738500	-0.26811700	-2.04833800
79	-0.08073000	-1.94724900	2.79002700
79	3.22041100	-2.00737900	-1.45520800
79	-0.11831500	2.16352200	-1.39125200
79	0.30712400	0.69202600	1.54459000
79	2.97486400	0.38921000	0.29175100

79	2.08245100	2.78996800	1.02590100
79	-4.14964600	-0.83038700	-0.61874200
79	-1.71968200	-1.51936400	0.63863600
79	-2.81975000	1.21020500	0.55597000
79	1.17156600	-2.04304800	0.33324400
79	-1.65889500	-0.11437400	-2.00206700
16	-0.87281400	3.88207200	0.39076200
8	-1.36345100	2.51300100	1.41455800
8	0.57334100	4.38712300	1.11684900

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SO<sub>2</sub>\_Au<sub>13</sub>  
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79	3.21059300	2.15625800	-0.52500000
79	0.52203600	-2.34436300	0.48990700
79	-1.53363600	-0.60326300	1.65814500
79	1.53459900	1.74376600	1.56553500
79	-2.32053400	1.90672600	-0.25334500
79	-0.29994000	3.72332200	-0.06096500
79	-4.13595300	-0.15071900	-0.33518000
79	0.83671500	-1.13056800	-2.47505000
79	0.42404800	1.30784500	-1.23146200
79	-1.68724900	-0.72403200	-1.48153200
79	3.15169300	-3.10359900	0.58368100
79	-2.13125100	-3.00317400	0.59825700
79	2.73346000	-0.49309000	0.03927600
16	-0.93131900	1.98129600	3.92143800
8	0.65872700	1.82826800	3.53598700
8	-1.80381000	1.26867600	2.72001100

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SO<sub>2</sub>\_Au<sub>14</sub>  
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79	-1.46244600	-2.36132100	-1.58893000
79	-3.56306400	1.45405800	0.79851000
79	-0.05102100	-1.96484200	1.90909100
79	-1.99508400	0.36449800	-1.37615800
79	-0.04195500	2.20924300	-2.30802800
79	-0.86837900	0.68738600	1.64734500
79	1.53921000	-3.05540300	-0.68699000
79	-1.27385300	3.18495900	0.11199800
79	0.75108300	-0.43167600	-1.49475500
79	1.80547000	0.04183000	1.79736100
79	1.49022900	2.39130800	0.12693400
79	3.34497200	-1.09516300	-0.63306700
79	4.01901300	1.47477900	0.72496100
79	-3.12431600	-1.30134800	0.71512300
16	-1.20186900	-4.12202900	1.11716400
8	-2.74241200	-3.44521400	0.78494100
8	-0.48120700	-4.09402200	-0.48530400

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SO<sub>2</sub>\_Au<sub>15</sub>  
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79	1.52193000	4.08833600	0.10541200
79	1.42791200	-0.57014100	-1.45863300
79	1.05173400	1.99116900	1.75225500
79	0.02893800	1.92260700	-1.13311000
79	2.62579600	-3.32477900	-0.18553000
79	1.65172600	-1.47926800	1.50757200
79	-1.29656800	-0.47672900	-1.35957200
79	-2.15360700	1.88707800	1.15200800
79	-2.94150400	2.43832500	-1.32880100
79	-0.16725800	-3.21676300	-0.14015600
79	-3.96213200	-0.14460900	-0.29376700
79	-1.81063800	-1.47529600	1.62360100
79	-2.91124300	-2.82431300	-0.47379800
79	3.01019800	1.74674900	-0.44988800

79	4.14698900	-0.68758000	-0.62116200
16	-0.80457600	-0.12736800	3.47317600
8	-1.39018300	1.43742800	3.12599300
8	0.80438200	0.05379200	2.80040400

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SO<sub>2</sub>\_Au<sub>16</sub>  
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79	-2.89198200	-0.83927700	-1.43421200
79	-3.22933600	1.96145100	-1.59196400
79	4.03430300	0.68548000	-0.32155400
79	2.39338400	0.81174000	1.95681800
79	4.20593700	-1.94030900	-1.38890300
79	2.37478800	-1.91088700	0.80818900
79	0.37271100	-1.19122600	2.47520100
79	1.84520700	2.44678100	-0.30438300
79	1.78593000	-0.50493600	-1.84653700
79	-0.46440400	2.36311300	1.55011100
79	-0.26409400	-1.86026500	-0.48256800
79	-2.67607000	-2.14877400	1.30529900
79	-2.56664100	-3.65428100	-0.89506800
79	-3.06922100	0.95159900	0.91200500
79	-0.50420100	0.90782500	-1.35699000
79	-0.61654000	3.81172500	-0.76183200
16	-1.55809600	-0.03566300	3.78086200
8	-1.24769400	1.58667500	3.38521500
8	-2.84260700	-0.42673200	2.64488100

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SO<sub>2</sub>\_Au<sub>17</sub>  
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79	3.44380400	-1.69220800	0.52842700
79	-3.84700500	-0.66200600	-0.98266600
79	-1.87379400	1.30169300	-1.48178100
79	-2.78890000	0.68978000	1.49278700
79	-2.10058600	3.33007800	0.50373600
79	-1.38779600	-1.49640200	-2.26752700
79	-1.66548200	-1.82689800	0.57759000
79	0.24955900	2.97800300	-1.20927100
79	-0.23419400	1.82074600	2.09630200
79	0.54494800	0.63338800	-2.89391100
79	-0.91988200	-0.94253800	3.09809500
79	2.31115400	2.34214300	1.10174100
79	-0.36255800	-3.86266700	-0.98425800
79	1.38115000	-1.68631600	-1.37467800
79	0.91186900	-2.70210700	1.59171100
79	3.08133500	0.41073000	-1.46843300
79	1.84381400	-0.03155500	2.28513400
16	3.68638500	3.84554000	-1.73375000
8	4.20508400	2.30344700	-1.88339900
8	2.37123200	3.79231000	-0.70246100

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SO<sub>2</sub>\_Au<sub>18</sub>  
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79	-3.05096300	-2.37614400	-0.49188000
79	-0.58654400	1.45128500	-2.01664900
79	2.27315400	2.37670600	-1.41408400
79	-3.23193400	0.19689800	-1.76988200
79	1.06228000	-1.77547700	1.25271800
79	3.51924100	-0.22501500	0.35173200
79	-1.58293500	-2.38477700	2.24360600
79	-2.05579500	0.13005600	0.81306200
79	0.16530300	3.69971000	-0.31861000
79	-2.73799100	2.72203800	-0.49013900
79	1.27138500	1.63350600	1.24454800
79	-0.41677300	0.03334700	3.13046500
79	2.68300900	-0.15894500	2.95516900

79	-1.26309800	2.57869800	2.24112100
79	-0.76690400	-1.37506000	-2.01122900
79	1.95912600	-2.64571100	-1.40035800
79	-0.29603000	-3.69218300	-0.29979500
79	1.43754900	-0.09246300	-3.09273000
16	4.45336600	-0.27748700	-1.95980200
8	3.64525600	1.10746300	-2.60786300
8	3.42498700	-1.50511600	-2.62728400

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SO<sub>2</sub>\_Au<sub>19</sub>  
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79	2.46352600	1.58578900	-1.37815600
79	-2.48902800	4.20174600	-1.46826800
79	4.94019000	-0.00019700	-1.12925900
79	0.98835300	1.67721000	1.01770900
79	-1.87412100	3.03018800	0.98978400
79	-0.10044700	-0.00086300	-1.67612700
79	-2.68522100	1.37734600	-1.47403800
79	3.50832100	-0.00075500	1.15015200
79	2.46284500	-1.58617200	-1.37929200
79	-0.98089900	1.64789600	3.16394300
79	-1.85051100	0.00078600	0.93447100
79	1.73043800	-0.00006200	3.30987500
79	0.98728700	-1.67718600	1.01706100
79	-2.68591200	-1.37724700	-1.47331900
79	0.10849400	-3.02538000	-1.31516800
79	-0.98066800	-1.64641200	3.16437600
79	-1.87441800	-3.02894300	0.99033300
79	-2.49019000	-4.20189800	-1.46689400
79	0.10856200	3.02372100	-1.31581000
16	1.88093700	0.00111100	-4.58341500
8	2.92303100	-0.00022600	-3.27553900
8	0.35990800	0.00229400	-3.96369400

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SO<sub>2</sub>\_Au<sub>1</sub>  
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16	-2.31318600	-0.01446800	0.00032000
8	-1.26218700	1.26994500	-0.00049200
8	-1.20661500	-1.26103400	-0.00050200
79	0.71849900	0.00202800	0.00003600

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SO<sub>2</sub>\_Au<sub>20</sub>  
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79	3.04752100	3.25749000	-2.38609000
79	0.88831600	0.11428500	5.01847000
79	-1.24087700	0.62714300	3.21600500
79	-3.17091100	1.02843000	1.31302500
79	0.86882500	-1.71760300	2.85844200
79	1.79782700	1.27178000	2.62031400
79	-0.42317000	1.82373400	0.67642900
79	-1.33750600	-1.27172000	0.94713700
79	-4.96236300	1.41649400	-0.83093100
79	1.74081600	-0.60779300	0.31035300
79	0.75035800	-3.33764700	0.64799500
79	-3.21526700	-0.76073700	-1.26277400
79	-2.31870000	2.22923000	-1.50776500
79	2.48141800	2.33459700	0.20916400
79	-0.42897200	-0.01905600	-1.96409300
79	-1.40745000	-2.78784800	-1.57588000
79	0.30531000	2.84092600	-1.97462200
79	1.58980600	-2.15043600	-2.17544600
79	2.45102300	0.45413800	-2.35306200
79	0.60886600	-4.76800400	-1.78414500
16	5.02568600	0.37056500	0.29948800
8	4.46684600	-1.07175200	0.64261300

8 4.98618900 0.61605900 -1.26652200

-----  
SO<sub>2</sub>\_Au<sub>2</sub>  
-----

79 1.45712600 -0.42051100 -0.01110300  
79 -1.45705200 -0.42064000 -0.01111800  
16 -0.00010400 2.48520500 -0.28039800  
8 1.30441100 1.66791100 0.39009000  
8 -1.30492500 1.66805000 0.39013900

-----  
SO<sub>2</sub>\_Au<sub>3</sub>  
-----

79 0.36562500 1.38638400 -0.00046900  
79 -1.96817500 -0.00092800 0.00041100  
79 0.36879700 -1.38637100 -0.00027700  
16 3.51922700 0.00267800 0.00114900  
8 2.57352500 -1.35396900 -0.00046500  
8 2.57133000 1.35764400 0.00147800

-----  
SO<sub>2</sub>\_Au<sub>4</sub>  
-----

79 -0.65368200 -1.72524000 -0.00178400  
79 -0.11340300 0.98210900 1.47789400  
79 -0.11594700 0.98624600 -1.47502600  
79 1.89610500 -0.35332700 -0.00176600  
16 -2.72832200 -0.20101400 0.00089200  
8 -2.27514400 0.74795000 -1.34384100  
8 -2.27231700 0.74242300 1.34878500

-----  
SO<sub>2</sub>\_Au<sub>5</sub>  
-----

79 0.00136800 -1.18982700 -0.00092300  
79 -1.68472100 1.15235200 -0.00221900  
79 -2.70308900 -1.31819900 0.00229400  
79 2.70616800 -1.31384700 -0.00228900  
79 1.68194600 1.15428100 0.00379900  
16 -0.00435900 4.21427400 -0.00387300  
8 -1.34686500 3.26664700 -0.00773600  
8 1.33908300 3.26779300 0.00893200

-----  
SO<sub>2</sub>\_Au<sub>6</sub>  
-----

79 1.19620800 1.26186700 -0.23400600  
79 -0.97625300 2.90545500 -0.13503800  
79 -2.00610800 -2.38692200 -0.24173300  
79 0.60067700 -1.59242200 0.11339600  
79 3.15574400 -0.59095800 -0.07436400  
79 -1.60692600 0.26773600 -0.52656700  
16 -0.72974200 0.74562900 2.75837000  
8 0.13693800 -0.55601700 2.52296400  
8 -2.26545800 0.40028800 2.80611500

-----  
SO<sub>2</sub>\_Au<sub>7</sub>  
-----

79 1.55891100 -0.00399600 0.71957900  
79 1.95882500 2.50912400 -0.52910800  
79 1.93716900 -2.44331000 -0.76255100  
79 -2.90898900 0.07149200 -0.87668300  
79 -1.64632800 -0.09329900 1.52171600  
79 -0.52699100 1.57184300 -0.69214600  
79 -0.52714000 -1.46904800 -0.88350000  
16 0.49046400 -0.40885800 4.17007800  
8 -1.03861600 -0.25741800 3.54042500  
8 1.58379500 -0.33506000 2.95851300



SO<sub>2</sub>\_Au<sub>8</sub>

79	-1.47570700	-1.48064400	-0.30446200
79	1.48532400	-1.47490400	-0.29699400
79	0.00581500	-3.42507300	0.92267300
79	3.52624500	0.05366600	-1.12834400
79	1.45515400	1.43154800	0.04115400
79	-1.46147400	1.42372600	0.04565600
79	-3.52538500	0.03942400	-1.12988300
79	-0.00793500	3.60000500	0.75977800
16	-0.00415200	-0.82458800	2.87881800
8	1.29596300	-0.00040600	2.50628000
8	-1.30777800	-0.00692000	2.50401100

SO<sub>2</sub>\_Au<sub>9</sub>

79	1.02410200	-2.52711600	0.75619600
79	0.95219500	-0.85030500	-1.40241400
79	0.40487200	1.71990700	-0.00127700
79	-2.36709200	0.78229200	0.26609100
79	-1.36822100	-1.88071600	-0.37326300
79	-4.04258900	-1.22146500	-0.42422500
79	-1.46601800	3.15621100	1.27569400
79	2.91035900	0.17118800	0.58699300
79	2.58673900	1.47341000	-1.77172500
16	3.61482700	-2.17675500	3.06633900
8	3.74776700	-0.69555300	2.34555300
8	2.50839400	-3.08206800	2.26509100

SO<sub>2</sub>

16	0.00000000	0.00000000	0.43444700
8	-0.00000000	1.30412600	-0.43444700
8	-0.00000000	-1.30412600	-0.43444700

**Table S3**

Vibrational Frequency which are computed by M06-2X/SDD method for CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, and SO<sub>2</sub> gases; isolated silver clusters Ag<sub>n</sub> (n=1-22), and gas/cluster structures at M06-2X/SDD level of theory

<b>CH<sub>4</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	1397.88	43.9087
2	1397.88	43.9087
3	1397.88	43.9087
4	1592.28	0.0000
5	1592.28	0.0000
6	3062.09	0.0000
7	3203.08	34.1139
8	3203.08	34.1139
9	3203.08	34.1139

  

<b>CO</b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	2106.02	111.4695

  

<b>CO<sub>2</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	637.36	38.4863
2	637.36	38.4863
3	1313.51	0.0000
4	2316.52	751.0493

  

<b>NO</b>		
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Mode	Frequency	Infrared
1	1879.14	50.6617

**NO<sub>2</sub>**

Mode	Frequency	Infrared
1	694.85	11.7535
2	1308.79	1.3403
3	1557.82	398.9807

**SO<sub>2</sub>**

Mode	Frequency	Infrared
1	428.86	40.4672
2	982.55	7.2307
3	1089.22	98.2766

**Ag<sub>2</sub>**

Mode	Frequency	Infrared
1	154.43	0.0000

**Ag<sub>3</sub>**

Mode	Frequency	Infrared
1	18.22	0.6613
2	119.55	1.7828
3	176.14	0.6251

**Ag<sub>4</sub>**

Mode	Frequency	Infrared
1	31.86	0.1720
2	58.75	0.0000
3	68.42	2.4081
4	87.20	0.0000
5	127.57	7.9557
6	152.07	0.0000

**Ag<sub>5</sub>**

Mode	Frequency	Infrared
1	24.08	0.0000
2	25.75	0.0387
3	59.00	0.2364
4	62.23	0.1800
5	79.92	0.0494
6	96.10	0.0002
7	113.12	0.0587
8	123.24	0.2823
9	146.07	2.9297

**Ag<sub>6</sub>**

Mode	Frequency	Infrared
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1	25.88	0.0000
2	25.88	0.0000
3	26.05	0.0786
4	60.11	0.1022
5	60.11	0.1023
6	74.04	0.9769
7	74.04	0.9770
8	100.61	0.0000
9	108.46	0.0000
10	118.51	0.0000
11	153.85	5.9003
12	153.85	5.8991

---

**Ag<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	38.68	0.0000
2	38.68	0.0000
3	63.01	0.2228
4	63.02	0.2228
5	68.60	0.0000
6	75.25	0.0000
7	75.25	0.0000
8	77.43	0.1132
9	84.96	0.0000
10	84.96	0.0000
11	94.53	0.0000
12	94.53	0.0000
13	120.76	0.0183
14	120.76	0.0183
15	125.73	0.0000

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**Ag<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	39.80	0.0000
2	46.02	0.2415
3	47.70	0.0000
4	56.00	0.2361
5	56.00	0.2361
6	57.71	0.0000
7	62.55	0.0000
8	65.45	0.0003
9	65.45	0.0003
10	73.72	0.0000
11	91.23	0.0377

12	91.23	0.0377
13	91.99	0.0000
14	102.27	0.0000
15	117.04	0.0035
16	117.04	0.0035
17	119.92	0.0000
18	127.94	0.0108

**Ag<sub>9</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	35.62	0.0031
2	40.36	0.0230
3	43.49	0.0510
4	46.30	0.0950
5	52.49	0.0864
6	52.75	0.0219
7	54.76	0.1454
8	61.94	0.0480
9	64.87	0.0017
10	65.31	0.0280
11	70.19	0.0027
12	73.43	0.0399
13	86.47	0.0354
14	87.09	0.0005
15	91.29	0.0499
16	94.59	0.1591
17	104.58	0.1362
18	113.39	0.0724
19	115.13	0.0028
20	124.43	0.3356
21	132.03	0.3825

**Ag<sub>10</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.02	0.0829
2	27.66	0.0256
3	27.75	0.1615
4	34.85	0.0000
5	44.60	0.0938
6	48.81	0.0329
7	52.20	0.0277
8	53.60	0.3778
9	56.91	0.5877
10	60.40	0.0432

11	66.74	0.0518
12	67.93	1.0524
13	73.59	0.0270
14	77.37	0.1000
15	81.86	0.1168
16	84.91	0.0222
17	89.43	0.0026
18	98.68	0.6558
19	106.66	0.4679
20	110.25	0.0093
21	120.75	0.2631
22	125.24	3.0256
23	134.37	2.0775
24	145.91	4.8680

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**Ag<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.42	0.0011
2	32.02	0.0674
3	34.05	0.0517
4	41.14	0.0000
5	42.70	0.0095
6	44.86	0.0000
7	49.33	0.0259
8	57.71	0.0001
9	58.51	0.0119
10	61.17	0.0000
11	63.73	0.1465
12	66.93	0.2598
13	74.07	0.2773
14	74.61	0.0196
15	75.43	0.0000
16	77.08	0.0014
17	80.12	0.0669
18	91.55	0.0000
19	94.38	0.0416
20	97.25	0.0259
21	100.26	0.0352
22	108.95	0.0001
23	110.52	0.0069
24	114.26	0.0142
25	116.60	0.0458
26	120.03	3.8634

27	130.98	0.0763
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<b>Ag<sub>12</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.57	0.0156
2	34.86	0.1270
3	35.16	0.1352
4	40.11	0.0080
5	42.10	0.0112
6	44.50	0.0413
7	46.10	0.0012
8	52.73	0.1076
9	54.23	0.0397
10	54.89	0.0788
11	58.47	0.5240
12	60.64	0.0001
13	64.66	0.1395
14	69.22	0.0082
15	71.05	0.2591
16	71.31	0.2416
17	76.80	0.1641
18	79.13	0.2130
19	80.68	0.0262
20	82.44	0.0339
21	93.39	0.0957
22	95.58	0.0031
23	100.80	0.0425
24	104.52	0.0166
25	109.94	0.3281
26	116.21	0.7961
27	121.47	0.0982
28	124.88	0.4391
29	127.07	0.3084
30	131.28	0.8610

<b>Ag<sub>13</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	29.78	0.0011
2	33.59	0.1018
3	34.13	0.0259
4	40.78	0.0026
5	44.50	0.0624
6	44.71	0.0030
7	46.95	0.0491

8	49.65	0.0827
9	51.16	0.0765
10	54.51	0.3239
11	55.19	0.0017
12	58.49	0.0055
13	58.59	0.0694
14	61.82	0.0991
15	66.02	0.0302
16	66.81	0.0062
17	69.77	0.0163
18	74.21	0.0817
19	77.06	0.0165
20	79.60	0.0217
21	79.94	0.0037
22	85.88	0.1140
23	86.58	0.0026
24	93.76	0.0220
25	101.17	0.0025
26	104.53	0.0078
27	105.84	0.0157
28	111.63	0.1383
29	113.45	0.7135
30	123.16	0.1825
31	124.35	0.5271
32	130.72	0.5323
33	132.55	0.1752

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**Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.27	0.0346
2	24.20	0.0333
3	24.63	0.0002
4	33.05	0.0029
5	37.12	0.0946
6	41.11	0.1621
7	43.15	0.0199
8	47.72	0.0088
9	49.07	0.0475
10	51.18	0.0265
11	53.39	0.0022
12	57.60	0.5463
13	58.59	0.0158
14	59.14	0.0975



15	61.91	0.0063
16	62.07	0.2584
17	65.18	0.0115
18	68.77	0.0071
19	73.67	0.0002
20	76.11	0.0317
21	77.70	0.0458
22	81.88	0.0371
23	85.30	0.0055
24	85.73	0.1937
25	95.21	0.0017
26	101.56	0.2065
27	102.97	0.0319
28	106.03	0.0689
29	107.61	0.2816
30	109.72	0.0543
31	113.33	0.0445
32	114.58	0.5292
33	123.65	0.9342
34	126.76	1.4148
35	134.23	0.4629
36	139.91	0.0003

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**Ag<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.06	0.0000
2	24.52	0.0001
3	30.52	0.0071
4	31.80	0.0001
5	36.46	0.0000
6	41.82	0.0000
7	43.96	0.0287
8	44.91	0.0043
9	48.76	0.0457
10	51.99	0.1002
11	54.37	0.0496
12	54.55	0.0322
13	57.28	0.1445
14	57.72	0.0006
15	63.37	0.0000
16	65.65	0.0990
17	65.80	0.3202
18	69.83	0.0012

19	71.61	0.2982
20	72.00	0.0933
21	73.12	0.4563
22	73.22	0.0632
23	76.53	0.0000
24	76.59	0.0140
25	85.36	0.0000
26	89.47	0.0610
27	91.34	0.1252
28	95.05	0.1333
29	98.65	0.1789
30	101.82	0.0397
31	104.04	0.0000
32	107.48	0.0102
33	107.58	0.0065
34	109.85	0.0484
35	114.09	0.3515
36	118.93	1.1683
37	123.37	0.0462
38	124.22	0.0622
39	134.86	0.0824

**Ag<sub>16</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.86	0.0127
2	24.49	0.0510
3	29.52	0.0010
4	36.34	0.0392
5	37.09	0.0214
6	40.16	0.1132
7	42.60	0.0218
8	44.57	0.1208
9	47.33	0.2325
10	47.58	0.0002
11	50.78	0.1640
12	51.06	0.0146
13	52.97	0.1930
14	55.33	0.0016
15	56.34	0.5468
16	58.20	0.0310
17	60.36	0.0579
18	61.75	0.0009
19	64.23	0.0199

20	66.22	0.1328
21	69.51	0.0009
22	71.18	0.0005
23	71.19	0.0240
24	72.75	0.0457
25	75.07	0.1168
26	83.68	0.1049
27	84.09	0.0022
28	90.31	0.0572
29	90.59	0.0736
30	91.69	0.0889
31	97.60	0.0023
32	101.42	0.0750
33	103.43	0.0577
34	108.20	0.2179
35	109.99	0.2589
36	114.29	0.0020
37	114.33	0.7139
38	117.57	0.0127
39	119.81	0.1150
40	124.39	0.0791
41	126.27	0.0851
42	134.94	0.0155

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**Ag<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.95	0.1415
2	20.80	0.0000
3	21.93	0.3855
4	33.46	0.6544
5	35.54	0.0234
6	37.96	0.0262
7	39.78	0.2870
8	40.21	0.1339
9	41.92	0.0000
10	43.15	0.0026
11	47.11	0.0000
12	51.55	0.0159
13	55.05	0.5304
14	55.63	0.0881
15	56.52	0.0000
16	57.40	0.0226
17	58.05	0.0587

18	62.32	0.2858
19	65.43	0.6363
20	66.13	0.0000
21	66.68	0.0197
22	67.26	0.1665
23	73.94	0.0000
24	74.06	0.1850
25	75.93	0.0506
26	79.21	0.0095
27	80.29	0.0887
28	84.39	0.0010
29	84.75	0.1342
30	91.63	0.0062
31	96.72	0.0090
32	96.92	0.0139
33	103.14	0.0836
34	105.78	0.0000
35	106.58	0.0017
36	110.49	0.0006
37	110.53	0.0000
38	110.73	0.0019
39	113.84	0.0943
40	115.32	0.1267
41	119.44	0.0000
42	120.82	0.0112
43	124.81	0.5123
44	126.23	0.5263
45	130.67	0.0224

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**Ag<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.64	0.0881
2	18.72	0.0056
3	24.05	0.4310
4	33.12	0.4562
5	34.18	0.0188
6	35.70	0.0456
7	37.65	0.0003
8	39.48	0.0710
9	40.87	0.1282
10	41.75	0.0462
11	47.58	0.0536
12	48.49	0.2254

13	49.32	0.0074
14	53.38	0.0052
15	54.20	0.0747
16	56.29	0.0296
17	59.84	0.1901
18	60.63	0.0101
19	65.42	1.3232
20	66.20	1.9842
21	66.85	0.3662
22	69.23	1.2976
23	69.64	0.7770
24	70.07	0.0134
25	70.72	0.1101
26	73.54	0.0078
27	75.81	0.1538
28	77.08	0.0000
29	83.48	0.1755
30	84.15	0.2281
31	86.13	0.0419
32	92.73	0.0224
33	93.68	0.0042
34	97.50	0.0967
35	100.26	0.0090
36	100.58	0.0870
37	106.14	0.9344
38	107.94	0.5079
39	109.23	0.6944
40	109.54	0.0118
41	111.83	0.1340
42	112.60	0.1460
43	113.68	0.0057
44	114.47	0.1092
45	114.65	0.4578
46	119.69	0.0239
47	121.68	0.0289
48	123.56	0.0059

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**Ag<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	31.46	0.0034
2	34.91	0.0205
3	37.44	0.0018
4	37.61	0.0312

5	39.17	0.0001
6	39.53	0.0000
7	39.62	0.0225
8	41.68	0.0471
9	42.52	0.0229
10	43.60	0.0155
11	45.72	0.0013
12	47.03	0.0056
13	47.26	0.0126
14	53.08	0.0070
15	53.15	0.0062
16	55.70	0.0223
17	56.05	0.0089
18	57.98	0.0660
19	59.33	0.2649
20	59.50	0.0294
21	60.72	0.1993
22	65.13	0.0095
23	65.21	0.0114
24	66.62	0.0216
25	67.32	0.0075
26	69.93	0.0442
27	72.25	0.0214
28	72.42	0.0137
29	74.44	0.0477
30	75.77	0.1142
31	78.29	0.0118
32	80.01	0.0124
33	80.22	0.0095
34	80.50	0.0048
35	84.51	0.0680
36	93.15	0.0215
37	94.21	0.0405
38	96.02	0.0209
39	97.55	0.0474
40	100.18	0.0003
41	104.31	0.1610
42	105.15	0.0086
43	106.88	0.0154
44	110.24	0.0000
45	118.54	0.1281
46	121.65	0.1404
47	133.31	0.2019

48	135.03	0.1953
49	136.80	0.5876
50	138.29	0.0018
51	143.07	0.1019

**Ag<sub>20</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.22	0.0403
2	31.18	0.0966
3	31.18	0.0966
4	39.77	0.0617
5	41.29	0.0125
6	41.29	0.0125
7	43.63	0.0059
8	44.90	0.0466
9	44.90	0.0467
10	50.08	0.0599
11	50.08	0.0596
12	52.14	0.0023
13	53.93	0.1307
14	53.93	0.1306
15	55.32	0.1804
16	57.42	0.0528
17	57.43	0.0530
18	59.64	0.0216
19	62.07	0.0211
20	62.07	0.0210
21	64.34	0.0266
22	64.42	0.0292
23	64.42	0.0293
24	66.33	0.0284
25	71.21	0.0014
26	71.25	0.0364
27	71.26	0.0363
28	72.30	0.0667
29	73.61	0.0227
30	73.61	0.0226
31	79.00	0.0336
32	79.00	0.0335
33	79.19	0.0418
34	87.31	0.0602
35	87.31	0.0607
36	90.44	0.0000

37	92.90	0.0123
38	93.55	0.0830
39	93.55	0.0830
40	95.82	0.0344
41	107.07	0.0924
42	107.07	0.0924
43	107.55	0.0042
44	109.51	0.0958
45	109.52	0.0950
46	111.99	0.0206
47	114.65	0.0506
48	114.65	0.0505
49	117.51	0.1284
50	127.27	0.0094
51	127.60	0.2446
52	127.61	0.2456
53	129.12	0.1202
54	129.13	0.1185

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**Ag<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	30.22	0.0235
2	30.28	0.0020
3	35.20	0.0000
4	36.56	0.1499
5	36.69	0.0000
6	40.35	0.0198
7	41.12	0.0040
8	41.84	0.0000
9	45.19	0.0959
10	46.60	0.0670
11	46.81	0.0064
12	47.14	0.0288
13	48.61	0.0000
14	49.80	0.0011
15	50.32	0.0023
16	50.86	0.0437
17	52.87	0.0000
18	55.34	0.0279
19	55.95	0.0002
20	56.17	0.0000
21	56.76	0.0510
22	57.38	0.5092



23	58.57	0.1483
24	59.60	0.0015
25	62.42	0.0002
26	63.12	0.2228
27	64.43	0.0000
28	69.67	0.1138
29	70.69	0.0058
30	71.08	0.0000
31	72.66	0.1448
32	73.08	0.0599
33	73.20	0.0263
34	76.47	0.0022
35	78.98	0.0005
36	84.23	0.0522
37	87.49	0.0073
38	89.12	0.0079
39	89.93	0.0000
40	91.76	0.1406
41	94.44	0.0000
42	96.87	0.0044
43	97.33	0.0343
44	99.60	0.0285
45	101.01	0.0000
46	104.40	0.3977
47	105.60	0.2598
48	106.76	0.0000
49	107.79	1.6572
50	109.28	0.0623
51	120.41	0.6331
52	121.69	0.2777
53	121.99	0.1610
54	124.10	0.0373
55	125.63	0.0000
56	127.98	0.3600
57	128.62	0.0722

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**Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.32	0.0056
2	26.40	0.0263
3	29.95	0.0432
4	30.66	0.0218
5	34.92	0.2261

6	37.73	0.1353
7	38.61	0.0623
8	40.59	0.0124
9	40.82	0.0593
10	43.64	0.0184
11	44.11	0.0491
12	45.45	0.0265
13	46.49	0.0059
14	46.76	0.0781
15	49.21	0.0967
16	50.15	0.1147
17	50.75	0.0509
18	51.49	0.0279
19	52.84	0.1695
20	54.22	0.1830
21	55.46	0.0315
22	56.19	0.0031
23	56.80	0.0610
24	57.14	0.0385
25	61.06	0.0144
26	61.69	0.0083
27	63.39	0.0940
28	65.00	0.0698
29	66.05	0.0191
30	67.79	0.0517
31	69.04	0.0850
32	70.81	0.0907
33	70.99	0.0572
34	72.51	0.0695
35	75.57	0.0176
36	78.26	0.0088
37	78.38	0.2481
38	80.63	0.3587
39	81.66	0.0489
40	83.24	0.0226
41	84.06	0.0888
42	86.87	0.1594
43	88.67	0.0202
44	90.21	0.0074
45	91.90	0.0449
46	94.98	0.0108
47	98.47	0.0206
48	102.39	0.0504

49	104.87	0.1015
50	105.93	0.0582
51	109.72	0.1285
52	118.75	0.4809
53	119.96	0.6975
54	124.66	0.0195
55	125.74	0.0548
56	129.36	0.4148
57	130.77	0.1124
58	137.05	0.1683
59	142.35	0.0595
60	157.57	0.4316

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**CH<sub>4</sub>/Ag<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	60.16	1.8035
2	87.41	0.1607
3	129.24	0.1124
4	1379.65	95.6998
5	1393.09	35.9435
6	1394.02	36.0086
7	1584.68	2.5991
8	1587.01	2.6783
9	3051.99	1.6742
10	3186.97	22.3748
11	3187.97	22.2928
12	3197.00	65.4254

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**CH<sub>4</sub>/Ag<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.27	0.2386
2	21.57	0.2381
3	108.52	11.8332
4	125.62	0.0119
5	132.48	0.0402
6	163.28	6.0045
7	1375.06	192.1018
8	1396.14	32.9550
9	1397.00	33.3977
10	1589.89	5.2383
11	1590.39	5.3143
12	3038.80	19.6587
13	3168.65	13.5568
14	3169.64	13.6325

15	3187.09	87.1957
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**CH<sub>4</sub>/Ag<sub>3</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.04	0.1675
2	16.45	0.2119
3	20.86	0.8464
4	26.40	0.4572
5	80.10	9.6206
6	112.47	2.4735
7	131.20	0.0313
8	136.51	0.0171
9	145.30	0.4281
10	1376.99	142.7721
11	1392.58	25.1880
12	1395.87	28.1120
13	1586.50	6.9279
14	1588.60	6.7694
15	3040.59	11.9599
16	3168.25	12.1466
17	3174.04	16.4463
18	3188.05	70.2500

**CH<sub>4</sub>/Ag<sub>4</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.30	0.0769
2	14.90	0.0661
3	32.95	0.1198
4	34.84	0.1322
5	55.17	0.0043
6	67.47	2.4025
7	74.55	10.2551
8	91.73	8.8349
9	128.96	2.2159
10	130.58	0.0919
11	138.71	0.0038
12	153.40	0.2618
13	1380.58	255.4308
14	1392.60	31.8526
15	1393.10	30.8959
16	1587.54	4.3804
17	1589.73	3.5337
18	3046.91	9.0607
19	3179.91	15.6925

20	3181.87	18.2192
21	3189.80	151.9683

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**CH<sub>4</sub>/Ag<sub>5</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.46	0.1201
2	15.60	0.0895
3	26.35	0.0313
4	26.73	0.0010
5	43.48	0.0053
6	57.44	0.4362
7	60.85	0.6110
8	79.33	0.2416
9	88.96	5.1125
10	96.77	4.1641
11	118.18	2.6402
12	122.15	2.3492
13	136.15	0.0108
14	144.12	0.0014
15	146.78	2.6143
16	1379.41	181.9008
17	1392.09	28.5264
18	1395.35	27.1124
19	1587.82	4.7583
20	1590.62	4.9212
21	3041.40	12.9575
22	3169.05	17.1789
23	3176.04	16.5569
24	3188.27	95.5467

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**CH<sub>4</sub>/Ag<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.40	0.2071
2	13.44	0.2320
3	25.76	0.0181
4	26.15	0.0455
5	26.72	0.0000
6	30.49	0.0011
7	58.28	0.0920
8	60.97	0.1968
9	72.51	0.1320
10	73.12	1.0335
11	91.83	9.6976
12	107.47	5.9418

13	111.76	12.7815
14	117.08	0.0125
15	130.06	0.0587
16	137.46	0.0376
17	153.42	6.2548
18	157.29	0.1592
19	1375.25	258.9207
20	1395.02	30.6307
21	1395.55	29.2106
22	1588.17	6.8296
23	1589.50	4.7239
24	3040.61	21.7304
25	3171.58	11.6538
26	3172.09	14.7464
27	3187.17	126.9280

**CH<sub>4</sub>/Ag<sub>7</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.19	0.0479
2	11.40	0.0318
3	13.30	0.0210
4	36.62	0.0000
5	37.05	0.0000
6	61.84	2.8916
7	62.46	0.2144
8	63.03	0.2280
9	67.57	0.7255
10	74.53	0.0004
11	75.05	0.0003
12	83.90	4.7908
13	84.74	0.0025
14	84.92	0.0082
15	94.56	0.0001
16	95.02	0.0003
17	99.27	0.0254
18	114.95	0.1130
19	120.34	0.0172
20	120.87	0.0223
21	125.82	0.4031
22	1380.14	145.3132
23	1390.46	24.0631
24	1391.10	23.6483
25	1586.68	6.2014

26	1587.53	6.0436
27	3045.69	3.4477
28	3178.25	12.3581
29	3180.15	12.0520
30	3188.09	95.4297

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**CH<sub>4</sub>/Ag<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.76	0.1502
2	15.29	0.1916
3	19.50	0.0145
4	40.02	0.0030
5	45.61	0.2957
6	49.90	0.0293
7	55.51	0.2647
8	56.18	0.2319
9	57.21	0.0088
10	62.35	0.0143
11	64.89	0.0008
12	65.27	0.0056
13	74.60	0.0668
14	90.94	0.0238
15	91.15	0.0199
16	92.44	0.0078
17	98.07	7.8922
18	102.83	0.2390
19	116.54	0.0059
20	117.86	0.3244
21	124.39	1.5357
22	132.89	6.3027
23	136.52	0.0014
24	151.42	0.9242
25	1378.16	195.2066
26	1392.73	27.5447
27	1394.77	23.4818
28	1588.17	6.4283
29	1589.09	8.1074
30	3039.52	16.3606
31	3168.08	10.5631
32	3172.03	11.3337
33	3185.94	101.5865

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**CH<sub>4</sub>/Ag<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
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1	2.61	0.0632
2	17.74	0.0357
3	35.00	0.0020
4	39.32	0.0656
5	40.53	0.0122
6	43.16	0.0810
7	45.62	0.0905
8	51.91	0.2081
9	52.73	0.0359
10	54.17	0.1200
11	60.00	0.1735
12	62.68	0.0036
13	65.73	0.0459
14	68.67	0.9732
15	71.01	0.0471
16	81.54	2.9003
17	84.68	0.0025
18	87.32	0.0250
19	89.77	0.0590
20	91.10	0.6367
21	94.78	0.3347
22	105.34	0.0726
23	113.62	0.0993
24	116.34	0.0041
25	125.68	0.3198
26	127.75	0.0735
27	129.04	0.6199
28	1378.44	115.8970
29	1384.91	15.4059
30	1390.84	24.8478
31	1581.21	10.3572
32	1587.07	5.1638
33	3044.03	3.4999
34	3173.78	19.2856
35	3180.44	12.8937
36	3187.57	82.6773

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**CH<sub>4</sub>/Ag<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.07	0.0613
2	18.75	0.0848
3	24.84	0.0793
4	27.31	0.1248



5	29.03	0.0802
6	34.94	0.0002
7	41.05	0.0055
8	44.12	0.1086
9	48.25	0.0281
10	52.19	0.1146
11	53.16	0.3355
12	56.96	0.6424
13	60.66	0.0564
14	66.54	0.0835
15	68.07	1.0621
16	72.87	0.0745
17	77.09	0.1400
18	81.17	0.0780
19	85.03	0.0385
20	89.31	0.0583
21	98.86	0.4775
22	99.27	0.4439
23	106.23	0.2241
24	109.57	0.3954
25	114.04	3.7825
26	115.39	2.6967
27	122.38	3.0081
28	132.28	6.3376
29	134.94	0.5453
30	145.65	5.0012
31	1378.30	140.2764
32	1389.69	17.8301
33	1391.33	19.1635
34	1584.86	7.0154
35	1586.95	6.8602
36	3038.18	13.3541
37	3164.57	9.6815
38	3170.15	14.1250
39	3183.67	78.1671

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**CH<sub>4</sub>/Ag<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.76	0.0887
2	21.34	0.0030
3	23.87	0.0391
4	32.54	0.0636
5	35.49	0.0593

6	41.08	0.0493
7	42.66	0.0415
8	45.62	0.0014
9	49.41	0.0212
10	51.80	0.0061
11	57.47	0.0100
12	58.42	0.0174
13	61.07	0.0048
14	62.51	0.1200
15	66.88	0.3065
16	73.08	0.1614
17	74.94	0.0856
18	75.47	0.1287
19	78.17	0.0460
20	79.91	0.0893
21	90.81	1.7881
22	91.66	0.3909
23	97.28	0.3120
24	98.78	2.6224
25	101.05	1.5485
26	109.05	0.0621
27	111.48	0.7061
28	114.14	0.5270
29	116.82	0.4769
30	120.33	3.2853
31	123.36	0.1610
32	130.95	0.1078
33	135.70	0.0835
34	1382.35	126.6307
35	1387.84	16.4494
36	1391.23	21.4913
37	1584.48	8.2864
38	1588.28	6.4231
39	3041.15	6.6905
40	3168.08	13.6574
41	3176.59	10.8853
42	3185.40	83.7168
<b>CH<sub>4</sub>/Ag<sub>12</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.09	0.1512
2	22.80	0.0802
3	23.50	0.0259

4	34.68	0.1376
5	35.64	0.1350
6	40.54	0.0049
7	42.50	0.0072
8	44.28	0.0275
9	44.54	0.0494
10	46.56	0.0034
11	52.99	0.1432
12	54.28	0.0229
13	55.01	0.1133
14	58.74	0.4636
15	61.04	0.0128
16	66.49	0.1906
17	68.66	0.0053
18	71.06	0.3218
19	71.57	0.1334
20	76.66	0.1163
21	78.64	0.2665
22	80.12	0.0824
23	82.06	0.1571
24	89.92	1.5694
25	94.32	0.6631
26	98.15	1.7306
27	100.78	0.3986
28	103.59	0.0476
29	107.89	0.7278
30	113.73	3.0194
31	116.89	1.0803
32	122.51	0.5308
33	125.37	0.1151
34	127.35	0.0120
35	130.55	1.6564
36	132.23	0.8773
37	1376.53	127.1108
38	1387.05	23.3544
39	1392.43	26.4046
40	1582.99	9.1324
41	1586.71	6.9671
42	3037.97	12.4729
43	3161.45	12.5635
44	3172.81	17.1918
45	3185.87	73.3812

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**CH<sub>4</sub>/Ag<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.43	0.1671
2	14.20	0.1348
3	17.17	0.0593
4	30.57	0.0314
5	33.77	0.1137
6	34.45	0.0563
7	40.49	0.0050
8	44.98	0.0227
9	45.16	0.0763
10	47.72	0.0275
11	49.90	0.1000
12	51.22	0.1229
13	54.84	0.3519
14	55.37	0.0392
15	58.15	0.0214
16	58.58	0.0680
17	61.97	0.1094
18	65.83	0.0224
19	67.06	0.0049
20	69.26	0.0264
21	74.51	0.0854
22	76.77	0.1950
23	78.64	0.4084
24	79.89	0.0485
25	83.50	4.8829
26	86.54	0.2834
27	89.58	3.5528
28	94.88	2.7391
29	101.64	0.4061
30	104.01	0.0908
31	108.46	2.3117
32	111.79	0.6689
33	114.37	0.9694
34	123.55	0.5665
35	127.07	0.7846
36	129.61	0.5964
37	131.13	1.5756
38	132.80	0.5692
39	145.63	0.3928
40	1377.73	216.9392

41	1391.17	22.7802
42	1394.14	21.5819
43	1587.37	6.0779
44	1587.57	6.6429
45	3040.04	13.9506
46	3167.89	11.1729
47	3174.07	16.3348
48	3185.05	113.5115

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**CH<sub>4</sub>/Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.59	0.0460
2	19.98	0.0450
3	21.10	0.0066
4	23.69	0.0315
5	25.28	0.0179
6	32.74	0.0041
7	36.71	0.0808
8	41.40	0.1598
9	42.97	0.0146
10	48.09	0.0062
11	49.62	0.0693
12	50.90	0.0231
13	53.15	0.0019
14	54.97	0.1118
15	57.45	0.4756
16	58.44	0.0144
17	59.29	0.0876
18	62.13	0.2810
19	62.36	0.0220
20	65.35	0.0224
21	68.97	0.0061
22	73.25	0.0236
23	75.92	0.2056
24	77.87	0.1025
25	81.78	0.2207
26	83.39	1.0773
27	85.58	0.0913
28	88.48	1.9121
29	95.18	0.0107
30	99.61	0.3238
31	101.90	0.2192
32	103.68	0.6289

33	105.95	0.1253
34	107.92	0.1724
35	109.88	0.0733
36	113.38	0.0950
37	114.35	0.5334
38	123.73	0.9742
39	126.36	1.3155
40	133.02	0.2718
41	135.27	0.2533
42	140.19	0.0273
43	1380.88	101.6034
44	1385.71	11.8384
45	1389.35	18.8734
46	1581.47	8.7732
47	1586.51	5.6659
48	3042.07	2.3967
49	3168.31	10.0205
50	3177.82	47.1702
51	3187.86	47.3597

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**CH<sub>4</sub>/Ag<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.39	0.0863
2	8.20	0.0900
3	23.30	0.0000
4	24.83	0.0000
5	30.33	0.0055
6	31.65	0.0048
7	33.47	0.0002
8	35.50	0.0004
9	41.93	0.0000
10	43.58	0.0347
11	44.24	0.0256
12	48.64	0.0398
13	52.03	0.1597
14	54.03	0.0428
15	54.49	0.0288
16	56.78	0.0793
17	57.08	0.1848
18	62.57	0.0001
19	64.45	0.4977
20	65.50	0.1794
21	68.98	0.1802

22	71.14	0.0845
23	71.90	0.4491
24	73.14	0.1906
25	73.94	0.4002
26	76.43	0.0003
27	76.65	0.0254
28	85.44	8.0777
29	85.52	0.0605
30	89.11	0.0698
31	91.75	1.6442
32	96.56	1.0672
33	98.74	0.3038
34	101.97	0.6591
35	103.41	0.0001
36	107.49	0.0064
37	107.85	0.3329
38	110.21	1.1072
39	114.66	0.2842
40	119.15	0.7056
41	123.50	0.1742
42	124.03	0.0590
43	124.48	0.0649
44	135.07	0.0284
45	136.54	0.0106
46	1378.88	227.2371
47	1389.20	20.2582
48	1392.13	22.3793
49	1585.08	7.6934
50	1586.85	6.2921
51	3043.11	8.1183
52	3173.71	13.6803
53	3177.35	14.1297
54	3185.85	140.6473

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**CH<sub>4</sub>/Ag<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.17	0.1349
2	15.51	0.0976
3	20.64	0.0238
4	20.98	0.0114
5	24.13	0.0442
6	29.16	0.0011
7	36.19	0.0371

8	36.96	0.0158
9	40.42	0.1255
10	42.87	0.0297
11	45.38	0.0804
12	47.11	0.0026
13	48.16	0.2996
14	50.68	0.1184
15	50.98	0.0698
16	53.40	0.4023
17	53.77	0.0217
18	56.25	0.5881
19	58.61	0.0142
20	60.14	0.0102
21	60.94	0.0231
22	63.89	0.0317
23	66.17	0.1514
24	69.91	0.0053
25	70.36	0.0543
26	71.24	0.0786
27	72.24	0.0558
28	74.93	0.1119
29	82.66	0.6826
30	83.08	0.1224
31	86.32	3.1615
32	90.23	0.0480
33	90.53	0.1237
34	95.44	2.3756
35	99.75	4.7697
36	102.00	1.8379
37	103.58	0.2073
38	109.27	1.0707
39	110.46	1.4071
40	114.45	0.0349
41	116.76	0.7939
42	117.67	0.2449
43	118.02	0.0734
44	120.44	0.0834
45	124.84	0.0687
46	125.33	0.1069
47	134.88	0.6535
48	139.00	0.1270
49	1376.20	207.5626
50	1390.68	20.2333



51	1392.72	20.0656
52	1585.05	8.0455
53	1587.46	6.7966
54	3039.42	15.2638
55	3167.05	12.5672
56	3173.37	9.6213
57	3185.10	113.8310

**CH<sub>4</sub>/Ag<sub>17</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.14	0.0721
2	17.53	0.1204
3	17.91	0.2520
4	19.27	0.3315
5	19.80	0.0019
6	33.56	0.7175
7	35.15	0.0103
8	35.99	0.0088
9	37.89	0.0029
10	39.32	0.2563
11	39.97	0.1794
12	41.74	0.0002
13	43.11	0.0161
14	47.35	0.0000
15	51.29	0.0156
16	55.53	0.1729
17	55.61	0.5347
18	56.48	0.0009
19	57.88	0.0379
20	58.10	0.0696
21	63.05	0.2844
22	65.42	0.0012
23	66.04	0.5882
24	66.32	0.0256
25	67.52	0.1476
26	73.97	0.0705
27	74.36	0.1060
28	75.62	0.0858
29	78.66	0.0109
30	79.87	0.1972
31	83.79	0.3837
32	84.14	0.0738
33	89.89	3.3272

34	93.92	3.9022
35	96.98	0.0060
36	97.61	1.2289
37	103.99	0.3864
38	105.64	0.0003
39	106.04	0.1580
40	109.77	0.0011
41	110.76	0.0017
42	111.64	0.6946
43	115.28	0.8157
44	116.21	0.1588
45	120.11	0.0004
46	122.45	1.3826
47	124.90	0.4160
48	126.86	0.8446
49	131.24	0.0221
50	135.81	0.0012
51	143.29	0.0491
52	1380.45	184.3105
53	1390.13	22.3945
54	1392.76	20.6005
55	1585.99	7.2461
56	1587.13	6.1483
57	3041.09	8.1114
58	3169.91	11.8516
59	3174.99	11.8613
60	3184.90	114.2629

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**CH<sub>4</sub>/Ag<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.98	0.0598
2	16.23	0.0776
3	20.24	0.0468
4	21.20	0.0055
5	23.17	0.3507
6	33.10	0.1996
7	33.92	0.0772
8	36.54	0.2192
9	37.64	0.0558
10	39.37	0.0534
11	41.21	0.1409
12	42.00	0.1180
13	47.99	0.0834

14	48.37	0.2149
15	49.42	0.0171
16	53.71	0.0309
17	54.23	0.0590
18	56.56	0.0163
19	59.42	0.2642
20	61.16	0.0090
21	65.09	0.8700
22	65.25	1.9433
23	66.56	0.9851
24	69.34	0.5212
25	70.30	0.1532
26	70.61	1.2686
27	71.39	0.3988
28	71.72	0.0137
29	73.75	0.0328
30	76.35	0.1280
31	77.06	0.0182
32	83.39	0.3462
33	84.44	0.1995
34	86.08	0.0747
35	91.13	2.0660
36	92.82	0.3242
37	95.62	1.6519
38	97.58	1.4887
39	100.05	0.0180
40	101.75	0.5209
41	106.37	1.0487
42	108.30	0.4882
43	109.28	0.6843
44	110.06	0.0152
45	111.81	0.3497
46	113.15	0.0926
47	113.59	0.0060
48	114.75	0.1498
49	114.97	0.1339
50	117.80	0.0140
51	119.83	0.0147
52	121.95	0.0408
53	123.73	0.0220
54	145.58	0.1469
55	1382.24	135.7145
56	1388.01	18.3821

57	1389.33	20.8241
58	1584.77	7.3284
59	1586.24	7.5958
60	3043.59	4.0870
61	3175.21	9.4694
62	3176.83	8.1168
63	3184.93	116.5643

**CH<sub>4</sub>/Ag<sub>19</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.75	0.1295
2	14.06	0.0994
3	31.98	0.0031
4	32.79	0.0261
5	36.99	0.0013
6	37.14	0.0275
7	38.85	0.0205
8	39.37	0.0044
9	39.98	0.0011
10	41.78	0.0236
11	42.51	0.0360
12	43.47	0.0231
13	45.85	0.0006
14	47.07	0.0106
15	47.87	0.0155
16	52.81	0.0186
17	53.33	0.0097
18	55.65	0.0018
19	55.99	0.0263
20	57.57	0.0949
21	58.96	0.2668
22	59.72	0.0761
23	61.18	0.1692
24	64.88	0.0250
25	65.10	0.0221
26	66.67	0.0304
27	67.13	0.0295
28	69.75	0.0257
29	71.42	0.0538
30	72.34	0.0200
31	74.50	0.0454
32	75.74	0.0369
33	77.71	0.0686

34	79.84	0.0836
35	80.17	0.0117
36	80.32	0.0019
37	81.79	0.0021
38	83.59	0.2126
39	91.76	0.6855
40	94.67	0.0588
41	95.93	0.0341
42	97.61	0.0379
43	100.40	0.1600
44	103.66	0.1255
45	105.36	0.2354
46	107.24	0.0762
47	109.20	1.8786
48	112.94	9.1079
49	119.16	1.3675
50	122.40	1.6738
51	125.37	0.8268
52	131.48	0.0782
53	133.34	0.2159
54	134.83	0.1371
55	136.87	0.2867
56	139.42	1.7849
57	143.41	0.8729
58	1375.53	197.8683
59	1391.23	19.2018
60	1394.13	18.1204
61	1585.78	6.9465
62	1586.38	8.1590
63	3031.76	14.7169
64	3158.70	9.7022
65	3163.68	8.4754
66	3179.30	105.8869

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**CH<sub>4</sub>/Ag<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.01	0.0283
2	20.07	0.0746
3	21.10	0.0618
4	30.54	0.0877
5	31.26	0.0507
6	39.54	0.0554
7	40.97	0.0253

8	41.23	0.0212
9	43.08	0.0180
10	44.29	0.0405
11	44.66	0.0309
12	46.28	0.0020
13	49.22	0.0305
14	49.51	0.0459
15	52.03	0.0162
16	53.23	0.1403
17	53.89	0.2084
18	54.31	0.1585
19	57.30	0.0516
20	57.81	0.0742
21	59.43	0.0311
22	61.21	0.0179
23	61.25	0.0248
24	63.75	0.0167
25	64.07	0.0132
26	64.37	0.0390
27	65.46	0.0501
28	69.88	0.0234
29	70.67	0.0689
30	70.81	0.0338
31	72.29	0.0629
32	72.82	0.0477
33	73.10	0.0025
34	77.90	0.0330
35	78.39	0.0170
36	79.09	0.0619
37	86.41	0.3815
38	86.94	0.0763
39	89.63	0.5018
40	90.97	0.9502
41	92.38	0.0556
42	92.93	0.1248
43	94.57	0.2024
44	98.60	2.6076
45	102.74	2.1964
46	105.30	0.0259
47	106.45	0.1202
48	106.88	0.0068
49	108.48	0.0439
50	109.26	0.2364

51	110.35	0.1125
52	112.50	0.0959
53	114.50	0.0695
54	115.24	0.0535
55	117.54	0.1363
56	127.40	0.0153
57	127.72	0.1056
58	127.94	0.1459
59	129.32	0.3600
60	129.42	0.4733
61	1378.17	129.5630
62	1386.91	17.2859
63	1390.19	14.8476
64	1582.75	5.8895
65	1584.22	7.4551
66	3040.73	4.7890
67	3168.82	8.2662
68	3174.31	14.1468
69	3184.65	90.9087

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**CH<sub>4</sub>/Ag<sub>21</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.53	0.0855
2	16.70	0.0453
3	28.98	0.0044
4	30.31	0.0326
5	34.58	0.0002
6	35.94	0.2031
7	36.72	0.0037
8	40.02	0.0136
9	40.95	0.0106
10	41.52	0.0023
11	44.51	0.1184
12	45.27	0.1380
13	45.66	0.0118
14	46.90	0.0415
15	47.33	0.0103
16	48.26	0.0007
17	49.84	0.0039
18	49.95	0.0015
19	50.95	0.0674
20	52.77	0.0047
21	55.08	0.0264

22	55.39	0.0216
23	55.54	0.0436
24	56.63	0.0259
25	56.96	0.4548
26	58.12	0.1841
27	59.16	0.0251
28	61.78	0.0922
29	62.77	0.2554
30	63.72	0.0031
31	69.26	0.0992
32	70.00	0.0137
33	70.59	0.0072
34	72.29	0.2420
35	72.96	0.0469
36	73.30	0.1863
37	75.78	0.0102
38	78.74	0.1113
39	82.25	2.3397
40	85.00	0.8945
41	88.38	0.3226
42	89.22	0.6729
43	89.34	0.0058
44	92.35	0.1182
45	94.51	0.1394
46	96.72	0.0242
47	98.05	0.4548
48	98.58	0.0877
49	100.66	0.0022
50	104.29	0.2414
51	106.15	0.2517
52	106.69	0.0298
53	107.26	1.6281
54	109.12	0.1374
55	110.49	0.0332
56	120.85	0.6505
57	121.47	0.2157
58	122.20	0.1966
59	124.58	0.0676
60	125.08	0.0566
61	127.54	0.3493
62	128.81	0.0543
63	137.03	0.7571
64	1380.09	126.9612



65	1386.29	17.0535
66	1388.41	14.4434
67	1582.31	6.6376
68	1584.02	6.5936
69	3040.44	3.6054
70	3167.28	9.8887
71	3174.83	9.4490
72	3185.95	99.0365

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**CH<sub>4</sub>/Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.99	0.1974
2	15.99	0.0865
3	20.07	0.0070
4	27.43	0.0267
5	30.06	0.0466
6	30.43	0.0263
7	33.76	0.0317
8	35.57	0.3200
9	38.06	0.0642
10	38.56	0.1036
11	40.70	0.0702
12	41.30	0.0089
13	43.99	0.0412
14	44.39	0.0364
15	45.38	0.0038
16	46.71	0.0466
17	47.31	0.0288
18	49.31	0.0925
19	50.16	0.0972
20	50.74	0.0569
21	51.93	0.0177
22	53.30	0.2056
23	54.19	0.2038
24	55.37	0.0522
25	56.43	0.0365
26	57.11	0.0286
27	57.91	0.0268
28	61.21	0.0389
29	62.05	0.0221
30	64.28	0.0615
31	65.49	0.1502
32	66.17	0.0080

33	67.67	0.0258
34	69.74	0.1230
35	70.47	0.0699
36	71.40	0.0430
37	72.52	0.1116
38	74.83	0.2000
39	78.09	0.0578
40	78.43	0.1226
41	80.24	0.1676
42	81.28	0.2550
43	83.22	0.0141
44	84.25	0.1479
45	85.83	0.2543
46	88.48	0.0628
47	89.08	0.4199
48	90.85	0.0013
49	94.09	0.1132
50	98.46	0.1234
51	101.49	2.1056
52	102.70	1.3026
53	105.95	0.1717
54	108.13	3.7356
55	109.71	2.5732
56	118.72	0.6957
57	119.99	0.8358
58	121.37	0.2761
59	124.24	0.0165
60	126.64	0.3370
61	130.74	0.2676
62	131.39	0.5362
63	137.40	0.5868
64	143.09	0.5829
65	156.75	0.4270
66	164.33	1.8593
67	1377.73	152.4991
68	1386.40	21.1755
69	1396.54	14.9136
70	1584.02	5.8051
71	1588.13	8.7147
72	3034.66	10.3484
73	3155.13	10.6840
74	3173.87	14.0768
75	3184.64	83.1868

<b>CO/Ag<sub>1</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	92.44	5.6234
2	193.83	7.9787
3	1996.58	1269.4501

<b>CO/Ag<sub>2</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.23	0.0291
2	37.87	0.1825
3	43.59	0.1828
4	98.47	7.1240
5	165.96	5.3898
6	2090.33	296.9430

<b>CO/Ag<sub>3</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	27.36	0.7634
2	74.72	0.6555
3	83.69	2.7958
4	94.77	0.0095
5	134.89	1.0303
6	161.99	1.0169
7	163.16	3.1987
8	197.18	0.1514
9	1861.85	1363.0843

<b>CO/Ag<sub>4</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	24.66	0.0450
2	28.49	0.0698
3	37.41	0.0640
4	68.92	2.7707
5	80.63	0.0163
6	87.62	0.0825
7	129.29	7.3195
8	140.19	0.3299
9	186.71	2.7531
10	223.58	0.1911
11	229.17	1.8352
12	2105.84	1057.6383

<b>CO/Ag<sub>5</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.66	0.0001

2	20.74	0.5829
3	24.37	0.1186
4	31.69	0.5104
5	56.75	0.5033
6	62.84	0.1013
7	77.22	0.1633
8	93.69	0.6265
9	105.52	4.4511
10	112.12	0.5853
11	113.31	0.4638
12	124.81	3.3798
13	141.01	23.7807
14	170.53	39.7226
15	2124.78	604.6890

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**CO/Ag<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.07	0.0799
2	12.75	0.0855
3	24.08	0.0026
4	26.44	0.0220
5	28.94	0.1130
6	56.13	0.1387
7	57.84	1.1685
8	71.90	0.8320
9	73.02	0.9858
10	93.77	4.7307
11	99.79	1.0261
12	108.92	5.5124
13	111.90	0.8132
14	132.86	9.5998
15	145.49	6.3050
16	155.93	6.4243
17	160.04	2.4414
18	2109.27	497.5961

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**CO/Ag<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.52	0.0500
2	16.56	0.2778
3	36.20	0.0000
4	41.97	0.0199
5	60.36	0.0660
6	64.38	0.3443

7	68.68	0.0445
8	73.86	0.2567
9	74.46	0.2233
10	76.06	0.0749
11	81.60	0.1354
12	88.85	0.0011
13	89.57	0.0122
14	93.06	0.5266
15	114.00	0.5992
16	115.57	4.5556
17	122.28	0.3220
18	123.73	0.0717
19	137.65	6.4450
20	176.63	7.2480
21	2119.66	764.0368

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**CO/Ag<sub>8</sub>**

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Mode	Frequency	Infrared
1	7.18	0.0040
2	17.47	0.1802
3	38.37	0.1212
4	43.96	0.5482
5	51.88	0.0236
6	54.53	0.1214
7	54.95	0.2181
8	55.47	0.0345
9	61.59	0.0308
10	64.66	0.0045
11	67.77	0.3694
12	75.88	0.0036
13	90.34	0.0542
14	90.63	0.0150
15	93.91	0.0008
16	101.49	0.2127
17	109.90	0.7563
18	114.01	0.6413
19	115.09	0.2723
20	123.26	4.3106
21	124.72	0.8425
22	142.92	5.8576
23	186.41	19.9365
24	2119.76	788.0078

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**CO/Ag<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.19	0.0003
2	17.55	0.2403
3	30.47	0.0404
4	40.06	0.2340
5	44.62	0.0119
6	50.05	0.0737
7	50.33	0.0066
8	54.14	0.0001
9	59.06	0.0376
10	61.67	0.0920
11	63.58	0.0034
12	64.26	0.2077
13	68.25	0.0065
14	72.99	0.2252
15	84.67	0.1870
16	86.98	0.0248
17	92.13	0.0001
18	95.75	0.1222
19	102.86	0.5944
20	110.63	0.1995
21	111.28	0.0947
22	120.26	0.3918
23	126.68	0.4157
24	129.42	5.2916
25	139.54	2.3910
26	178.51	1.2255
27	2124.89	796.0614

**CO/Ag<sub>10</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.14	0.0513
2	15.97	0.0831
3	18.21	0.0595
4	27.51	0.1026
5	30.93	0.0986
6	35.12	0.0129
7	43.69	0.0343
8	46.82	0.1671
9	50.45	0.5694
10	51.62	0.0475
11	57.37	0.6942
12	63.67	0.1923

13	66.50	0.0693
14	69.48	1.3662
15	71.29	0.0761
16	77.38	0.1018
17	82.08	0.0664
18	87.79	0.0358
19	90.38	0.0195
20	99.13	0.5935
21	104.16	0.5518
22	110.79	0.0514
23	117.73	0.2620
24	122.63	2.5967
25	135.10	2.6502
26	146.75	5.0727
27	167.14	3.0344
28	181.28	0.3686
29	194.08	0.0676
30	2102.69	882.8171

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**CO/Ag<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.93	0.0140
2	23.58	0.1634
3	26.68	0.3224
4	34.34	0.1102
5	35.05	0.0602
6	40.21	0.0007
7	43.43	0.0047
8	45.95	0.0036
9	49.69	0.0170
10	56.91	0.0409
11	59.68	0.0104
12	60.45	0.0008
13	63.88	0.2034
14	67.36	0.6743
15	72.13	0.7041
16	72.86	0.2270
17	75.05	0.0198
18	76.37	0.0137
19	79.08	0.2866
20	81.93	0.2466
21	90.36	0.0004
22	91.90	0.0606

23	97.01	0.0270
24	97.33	0.3988
25	100.79	0.1368
26	109.18	0.0212
27	111.23	0.0923
28	115.97	0.0121
29	117.22	0.1180
30	119.91	4.7936
31	129.39	1.9221
32	134.18	1.9370
33	2039.96	95.0090

**CO/Ag<sub>12</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.54	0.0299
2	15.33	0.0387
3	23.68	0.0227
4	33.61	0.1259
5	36.14	0.1634
6	40.23	0.0752
7	43.37	0.0167
8	44.12	0.1037
9	50.77	0.0660
10	54.47	0.0992
11	57.39	0.1721
12	58.83	0.0828
13	59.81	0.2468
14	61.93	0.1557
15	65.21	0.2714
16	67.14	0.0357
17	70.72	0.1767
18	74.37	0.0174
19	76.24	0.1284
20	78.91	0.0989
21	80.01	0.1860
22	81.44	0.4742
23	90.79	0.6749
24	94.92	0.0004
25	98.62	0.0669
26	103.49	0.0410
27	108.67	0.2435
28	114.53	1.5129
29	119.75	0.1349



30	127.69	1.0766
31	129.22	0.7958
32	131.71	0.3341
33	134.97	6.7933
34	159.98	3.2452
35	186.36	1.6045
36	2119.51	786.6373

**CO/Ag<sub>13</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.62	0.0388
2	9.05	0.1136
3	30.40	0.0178
4	34.17	0.0420
5	34.62	0.0185
6	40.30	0.0189
7	44.08	0.0308
8	45.59	0.0232
9	46.33	0.2140
10	49.03	0.0587
11	49.79	0.2178
12	51.92	0.0112
13	54.13	0.6816
14	55.33	0.1512
15	57.62	0.9280
16	58.13	0.0534
17	58.30	0.4355
18	62.43	0.0814
19	65.51	0.0456
20	66.74	0.0061
21	69.02	0.2067
22	74.45	0.0836
23	77.60	0.0249
24	78.92	0.1279
25	79.78	0.0179
26	86.04	0.2378
27	86.74	0.1878
28	90.94	2.4880
29	96.45	4.3464
30	101.87	0.4548
31	103.66	0.1204
32	109.39	2.0570
33	111.94	1.1295

34	115.21	1.3742
35	123.36	0.7268
36	129.96	0.4235
37	132.48	0.3987
38	135.18	6.5810
39	2091.00	350.7435

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**CO/Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.32	0.0374
2	19.03	0.0120
3	30.20	0.0995
4	32.79	0.0127
5	38.53	0.1109
6	39.70	0.0500
7	43.08	0.1448
8	45.35	0.0953
9	48.13	0.0303
10	50.35	0.0575
11	52.64	0.2333
12	53.87	0.1903
13	55.28	0.1215
14	57.26	0.1290
15	59.32	0.0444
16	63.08	0.0186
17	64.22	0.1644
18	66.18	0.0038
19	66.86	0.0349
20	69.01	0.0567
21	72.93	0.0563
22	73.50	0.2868
23	74.85	0.1081
24	77.29	0.0845
25	84.21	0.0081
26	89.25	0.6633
27	94.91	0.1634
28	95.79	0.0497
29	98.89	0.2351
30	99.71	0.0659
31	102.70	0.1177
32	105.74	0.0490
33	116.09	0.4932
34	119.45	0.2992

35	120.11	0.5015
36	125.07	0.2805
37	135.26	0.6258
38	139.43	0.4036
39	163.71	2.1139
40	183.46	4.3711
41	197.58	0.0257
42	2114.49	951.7504

**CO/Ag<sub>15</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.03	0.1344
2	15.98	0.0073
3	23.05	0.0000
4	24.63	0.0128
5	31.72	0.0313
6	33.74	0.0002
7	36.25	0.0059
8	42.14	0.0240
9	43.59	0.1030
10	45.17	0.0021
11	49.12	0.0908
12	52.61	0.0243
13	53.03	0.0040
14	54.86	0.1370
15	56.57	0.1582
16	57.62	0.3106
17	59.12	0.1347
18	63.21	0.0261
19	64.31	0.2397
20	65.15	0.0554
21	65.89	0.2300
22	69.81	0.2093
23	70.85	1.4886
24	71.62	0.3726
25	72.49	0.3781
26	73.80	0.3839
27	77.18	0.0040
28	77.20	0.0618
29	82.07	6.6174
30	85.56	0.0017
31	89.47	0.0044
32	91.48	0.5782

33	95.41	0.0276
34	97.57	0.1745
35	102.49	0.8656
36	102.86	0.0008
37	108.08	0.0069
38	109.32	1.3487
39	109.57	0.0995
40	116.65	0.6780
41	119.20	1.3436
42	123.77	0.2514
43	125.28	0.1346
44	135.36	0.2610
45	2096.86	322.4147

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**CO/Ag<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.71	0.0042
2	14.96	0.1450
3	19.93	0.0075
4	23.85	0.0542
5	28.41	0.0127
6	35.61	0.0674
7	36.39	0.0710
8	40.21	0.2036
9	42.01	0.1194
10	43.30	0.4524
11	44.80	0.0861
12	47.64	0.1069
13	48.17	0.0895
14	49.34	0.1487
15	51.00	0.0209
16	52.90	0.1431
17	54.22	0.0870
18	55.86	0.4813
19	58.03	0.2090
20	59.13	0.0676
21	60.27	0.1060
22	62.49	0.0412
23	65.78	0.1646
24	67.56	0.1132
25	70.48	0.0347
26	70.94	0.0193
27	71.39	2.1529

28	71.69	1.2805
29	73.49	0.6990
30	78.76	4.7325
31	83.34	0.0198
32	85.13	1.1057
33	89.57	0.2961
34	90.66	0.0261
35	92.35	0.7416
36	97.71	0.0756
37	100.62	0.0547
38	103.94	0.1850
39	108.28	0.1104
40	109.84	0.2207
41	114.21	0.7397
42	114.87	0.3731
43	118.24	0.1175
44	120.62	0.1744
45	124.83	0.3651
46	127.01	0.1621
47	135.01	0.0565
48	2096.48	311.1861

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**CO/Ag<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.87	0.0087
2	16.36	0.0495
3	17.27	0.1226
4	19.37	0.3654
5	20.03	0.0213
6	33.47	0.5158
7	35.73	0.0585
8	37.88	0.0095
9	39.47	0.2066
10	39.74	0.1274
11	40.85	0.0765
12	43.31	0.0094
13	45.69	0.0858
14	50.92	0.1171
15	52.95	0.1945
16	54.02	0.3343
17	55.71	0.0049
18	56.07	0.4038
19	56.67	0.0427

20	57.55	0.0661
21	61.09	0.3454
22	62.54	0.2286
23	65.88	0.1236
24	66.00	0.4140
25	66.23	0.2373
26	67.97	0.2635
27	73.52	0.2113
28	73.84	0.0050
29	75.56	0.0402
30	78.81	0.0285
31	80.22	0.0837
32	83.29	0.7072
33	84.61	0.3924
34	86.48	1.9236
35	92.41	0.3194
36	96.97	0.0238
37	97.32	0.0776
38	102.82	0.1189
39	105.30	0.0419
40	106.61	0.0211
41	109.77	0.0047
42	110.31	0.0037
43	111.06	0.1082
44	113.91	0.0825
45	116.31	0.1050
46	118.51	0.0022
47	122.09	0.0581
48	124.34	0.4660
49	125.92	0.6251
50	130.85	0.0312
51	2099.21	253.6215

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**CO/Ag<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.67	0.4321
2	14.78	0.0153
3	19.03	0.3017
4	19.97	0.0369
5	28.20	0.1264
6	33.06	0.1494
7	36.57	0.0358
8	38.99	0.0388

9	39.27	0.1303
10	40.19	0.0019
11	40.65	0.0712
12	41.83	0.0793
13	46.01	0.0083
14	47.37	0.1523
15	47.56	0.0103
16	48.96	0.0012
17	53.26	0.0906
18	55.28	0.0447
19	57.85	0.0068
20	58.41	0.9396
21	61.32	0.1173
22	63.76	0.1899
23	64.03	0.3269
24	64.62	0.1975
25	66.82	0.0193
26	69.90	0.3543
27	73.24	0.3804
28	73.86	0.6931
29	76.26	0.2738
30	80.82	0.0236
31	84.10	0.2709
32	84.15	0.0066
33	88.07	1.4885
34	91.05	0.0518
35	91.84	0.0484
36	93.24	0.0293
37	101.05	0.0982
38	103.98	0.0129
39	106.40	0.1576
40	107.25	0.2061
41	108.48	0.0001
42	110.97	0.4298
43	113.23	0.0370
44	113.80	0.2579
45	115.50	0.2312
46	118.83	0.0070
47	120.11	1.1520
48	121.07	0.0239
49	124.52	0.1947
50	130.75	0.2252
51	160.84	3.2274

52	174.66	3.0063
53	192.45	2.2973
54	2117.18	1168.4333

**CO/Ag<sub>19</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.24	0.0256
2	18.23	0.0130
3	31.48	0.0107
4	33.61	0.2316
5	35.38	0.2582
6	36.99	0.0247
7	37.68	0.0597
8	39.02	0.0319
9	39.81	0.0000
10	41.30	0.0173
11	42.07	0.0406
12	42.95	0.0583
13	43.95	0.1261
14	45.97	0.0164
15	46.90	0.0055
16	47.51	0.0442
17	51.43	0.2564
18	53.06	0.0205
19	54.33	0.3262
20	55.59	0.0091
21	56.19	0.1899
22	57.75	0.0800
23	58.91	0.0717
24	59.65	0.2193
25	60.26	0.1545
26	63.61	0.5455
27	64.79	0.0712
28	65.32	0.0007
29	66.48	0.0749
30	68.70	0.5576
31	70.07	0.0725
32	72.27	0.0251
33	73.27	0.2056
34	74.62	0.0377
35	77.94	0.0142
36	79.31	0.0191
37	80.01	0.0160



38	80.68	0.1222
39	83.84	0.3359
40	85.77	2.3115
41	93.64	0.1873
42	94.66	0.2493
43	95.88	0.1790
44	97.80	0.0371
45	99.95	0.0051
46	104.13	0.2003
47	105.21	0.0615
48	107.07	0.0005
49	110.09	0.0037
50	118.43	0.1201
51	121.82	0.1261
52	132.96	0.2157
53	134.72	0.1636
54	136.21	0.1775
55	138.39	0.1614
56	143.85	0.1469
57	2099.49	262.3208

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**CO/Ag<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.57	0.0371
2	17.05	0.2515
3	32.84	0.0410
4	33.96	0.0880
5	35.15	0.0427
6	37.82	0.0913
7	38.08	0.0410
8	39.54	0.0191
9	44.10	0.0678
10	45.13	0.0253
11	46.17	0.0179
12	47.44	0.0745
13	47.72	0.0540
14	49.60	0.0253
15	50.20	0.0931
16	53.06	0.0197
17	53.58	0.0782
18	54.28	0.0418
19	54.98	0.0045
20	55.22	0.0428

21	57.74	0.0380
22	58.73	0.0441
23	60.32	0.0123
24	61.52	0.0104
25	62.07	0.0401
26	63.18	0.0368
27	64.64	0.0575
28	67.09	0.0942
29	71.42	0.1023
30	72.06	0.0200
31	74.50	0.2722
32	77.44	0.1433
33	78.28	0.0244
34	79.14	0.0486
35	79.86	0.0218
36	81.33	0.0566
37	82.05	0.1258
38	82.70	0.0708
39	84.18	0.0040
40	85.76	0.0591
41	91.26	0.0131
42	95.37	0.1964
43	95.74	0.0637
44	96.68	0.1387
45	102.60	0.0884
46	102.81	0.0391
47	106.83	0.1845
48	109.52	4.9753
49	117.76	0.2167
50	119.00	0.2491
51	121.69	0.2806
52	129.87	3.2472
53	132.87	1.2897
54	134.81	0.7010
55	135.30	0.7276
56	137.09	3.6511
57	140.59	0.2902
58	141.06	0.7746
59	167.44	12.6124
60	2125.06	748.7858

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CO/Ag<sub>21</sub>

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Mode	Frequency	Infrared
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1	8.78	0.0042
2	18.77	0.0154
3	28.26	0.0061
4	31.70	0.0387
5	34.23	0.0689
6	36.09	0.0964
7	36.55	0.0480
8	39.86	0.0030
9	40.58	0.0220
10	42.08	0.0095
11	43.29	0.0025
12	44.51	0.0579
13	45.96	0.0818
14	47.26	0.0457
15	48.37	0.0550
16	48.51	0.0621
17	49.46	0.0027
18	49.98	0.2976
19	50.94	0.0749
20	51.76	0.1660
21	53.08	0.0147
22	55.06	0.0577
23	55.57	0.2861
24	56.07	0.0029
25	56.45	0.0346
26	57.09	0.2000
27	58.25	0.1304
28	58.71	0.0944
29	62.37	0.0005
30	63.15	0.4041
31	63.86	0.0046
32	66.11	0.7881
33	70.16	0.0570
34	71.30	0.4410
35	71.33	0.0543
36	71.98	0.0328
37	72.61	0.0502
38	75.28	1.7943
39	77.13	0.5412
40	78.54	0.0009
41	84.10	0.0771
42	87.98	0.1263
43	89.18	0.0085

44	90.05	0.0003
45	92.50	0.4371
46	94.42	0.1643
47	95.82	0.0075
48	96.59	0.0022
49	99.28	0.0484
50	101.45	0.0000
51	104.33	0.3750
52	106.11	0.1722
53	106.26	0.0143
54	107.44	1.5606
55	109.30	0.0396
56	119.72	0.7687
57	121.44	0.1849
58	121.79	0.0448
59	123.91	0.0406
60	125.19	0.0011
61	128.03	0.2666
62	129.64	0.3043
63	2099.95	250.1474

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**CO/Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.96	0.0130
2	17.24	0.0970
3	18.85	0.0805
4	26.15	0.0373
5	29.39	0.0819
6	31.67	0.0651
7	34.58	0.1876
8	36.31	0.1354
9	37.46	0.0351
10	39.81	0.0653
11	41.58	0.0142
12	43.86	0.0131
13	44.79	0.0250
14	45.70	0.0471
15	46.76	0.0205
16	47.51	0.1098
17	48.68	0.0734
18	50.36	0.0443
19	51.15	0.0704
20	51.97	0.0291

21	53.63	0.0198
22	54.40	0.0725
23	55.32	0.2533
24	56.31	0.1416
25	57.66	0.0085
26	58.63	0.0856
27	61.24	0.0412
28	62.03	0.0215
29	63.43	0.1949
30	65.43	0.0145
31	65.82	0.0786
32	67.23	0.0327
33	69.28	0.1081
34	69.53	0.0442
35	70.81	0.1447
36	72.15	0.4904
37	75.14	0.1451
38	76.54	0.1112
39	78.77	0.1147
40	80.06	0.3911
41	81.41	0.0091
42	82.11	0.1125
43	84.31	0.1574
44	85.98	0.1789
45	87.97	0.1333
46	89.66	0.0207
47	89.81	0.0187
48	94.26	0.0068
49	98.79	0.0316
50	102.23	0.0138
51	103.72	0.0516
52	105.09	0.1604
53	109.54	0.1161
54	117.29	6.5757
55	119.10	0.5435
56	120.36	0.6371
57	124.61	0.1925
58	125.86	0.0469
59	129.07	0.6120
60	131.70	0.8001
61	132.47	0.7027
62	139.96	8.8266
63	143.93	0.4000

64	158.55	1.2254
65	173.75	14.3357
66	2118.69	916.8740

**CO<sub>2</sub>/Ag<sub>1</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.76	0.3782
2	65.18	2.7102
3	631.53	31.6143
4	633.49	33.2397
5	1311.02	0.0523
6	2309.86	904.0330

**CO<sub>2</sub>/Ag<sub>2</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.47	0.0478
2	42.72	0.2664
3	45.62	0.2888
4	92.43	6.8850
5	165.76	5.8438
6	625.95	33.2771
7	626.60	33.7894
8	1319.86	2.7999
9	2321.77	1272.6876

**CO<sub>2</sub>/Ag<sub>3</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.83	0.1099
2	10.35	0.0387
3	46.62	0.0940
4	46.96	0.9221
5	52.68	0.0161
6	100.81	1.8175
7	112.63	1.8911
8	164.88	11.1892
9	621.48	28.6334
10	625.03	33.0700
11	1323.07	3.9528
12	2326.79	1274.2616

**CO<sub>2</sub>/Ag<sub>4</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.39	0.2274
2	14.18	0.0074
3	30.73	0.2466
4	58.04	1.2854

5	58.68	0.0705
6	69.24	0.1637
7	70.93	1.2863
8	87.41	0.0252
9	126.22	7.0563
10	131.87	4.6671
11	175.56	7.8493
12	615.27	28.0614
13	622.45	29.3266
14	1323.08	4.5516
15	2327.15	1032.2318

**CO<sub>2</sub>/Ag<sub>5</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.92	0.0434
2	20.39	0.0162
3	25.90	0.0105
4	35.40	0.0459
5	38.28	0.0698
6	55.60	1.2107
7	58.30	0.2276
8	63.22	0.1145
9	78.56	0.0217
10	91.57	1.1896
11	96.18	0.2362
12	113.85	0.0486
13	123.35	0.2399
14	143.19	2.7914
15	589.14	66.5550
16	612.66	11.9809
17	1309.10	0.1418
18	2296.99	357.9770

**CO<sub>2</sub>/Ag<sub>6</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.47	0.0115
2	18.48	0.0221
3	22.38	0.0049
4	26.80	0.0330
5	35.55	0.0747
6	38.16	0.0476
7	45.87	1.2829
8	58.21	0.1219
9	59.96	0.1211

10	72.99	0.9595
11	73.97	0.9926
12	75.41	0.6488
13	101.09	0.0011
14	109.43	0.0295
15	117.08	0.0023
16	152.93	5.7510
17	153.54	5.6281
18	593.61	65.0571
19	612.43	12.6260
20	1308.70	0.0794
21	2294.46	335.7752

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**CO<sub>2</sub>/Ag<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.92	0.0000
2	23.31	0.3924
3	34.58	0.1355
4	36.97	0.0042
5	39.66	0.0115
6	52.86	0.9206
7	62.30	0.1849
8	63.77	0.1749
9	67.76	0.0669
10	72.61	0.5853
11	75.26	0.0026
12	75.88	0.5377
13	78.87	0.3060
14	85.33	0.0007
15	92.44	0.3808
16	93.72	0.0003
17	101.12	3.2034
18	120.97	0.0337
19	121.12	0.1907
20	126.01	0.4103
21	570.69	70.5415
22	603.84	11.4762
23	1308.25	1.4497
24	2296.33	295.5918

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**CO<sub>2</sub>/Ag<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.96	0.0061
2	7.46	0.0208



3	32.70	0.3788
4	38.89	0.4616
5	40.80	0.1581
6	47.58	0.3038
7	51.99	0.0973
8	54.85	0.1291
9	56.68	0.2697
10	57.38	0.0035
11	62.15	0.0201
12	64.51	0.1269
13	64.82	0.0180
14	75.93	0.0095
15	90.32	0.2205
16	90.80	0.5554
17	93.18	0.2592
18	95.09	5.0218
19	103.18	0.3039
20	116.36	0.0137
21	116.97	0.3072
22	124.83	0.7784
23	135.89	8.2616
24	623.31	25.7853
25	624.66	26.4411
26	1318.18	2.4468
27	2317.73	1556.1123

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**CO<sub>2</sub>/Ag<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.63	0.0980
2	9.18	0.3944
3	32.88	0.0651
4	38.92	0.0715
5	41.66	0.0919
6	44.25	0.1070
7	46.15	0.1851
8	49.88	0.1861
9	50.93	0.0237
10	54.60	0.0445
11	56.92	0.6038
12	62.60	0.0381
13	63.81	0.0509
14	66.14	0.1304
15	69.40	0.4296

16	73.13	0.0755
17	84.45	1.1379
18	86.00	0.0647
19	88.34	0.1207
20	93.01	0.6006
21	101.82	1.2896
22	108.31	1.3681
23	112.82	0.0631
24	118.09	2.0122
25	122.38	0.5525
26	133.19	0.5821
27	576.27	71.1288
28	607.30	14.1840
29	1308.40	0.6513
30	2297.69	375.3164

**CO<sub>2</sub>/Ag<sub>10</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.48	0.0753
2	8.74	0.0121
3	16.57	0.1013
4	27.64	0.1450
5	30.01	0.1909
6	35.39	0.0599
7	44.33	0.1770
8	46.03	0.2031
9	47.66	0.0874
10	51.49	0.1565
11	52.23	0.3003
12	55.66	0.5890
13	59.83	0.2424
14	62.85	0.4688
15	67.01	0.1386
16	67.54	1.2183
17	73.37	0.0458
18	77.56	0.2383
19	82.02	0.2017
20	83.41	0.1903
21	88.72	0.0187
22	98.57	0.7459
23	105.18	0.4360
24	110.52	0.0086
25	117.06	1.5683

26	122.07	3.1528
27	134.13	4.6531
28	139.19	2.8614
29	146.52	4.4249
30	580.48	84.4151
31	608.46	15.1173
32	1310.86	0.2473
33	2304.47	659.5949

**CO<sub>2</sub>/Ag<sub>11</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.50	0.6265
2	21.18	0.1975
3	24.22	0.0827
4	35.43	1.3927
5	37.56	0.7915
6	39.27	0.1004
7	40.78	0.0423
8	45.12	0.7094
9	49.34	0.3027
10	55.58	0.4225
11	56.05	0.1136
12	59.99	0.1460
13	64.32	0.5710
14	65.36	1.3230
15	68.89	0.4069
16	71.71	0.8544
17	77.88	1.0065
18	82.22	0.2839
19	84.46	0.1065
20	87.98	0.1873
21	91.95	0.0358
22	97.40	0.3590
23	101.74	0.5142
24	106.78	0.4145
25	113.71	0.1307
26	118.73	0.1207
27	121.94	2.9616
28	124.49	0.0636
29	128.93	0.4359
30	132.98	0.5709
31	168.89	2.3212
32	203.44	24.2793

33	360.15	1.3525
34	655.84	141.8471
35	1140.67	55.6280
36	1735.45	758.2835

**CO<sub>2</sub>/Ag<sub>12</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.26	0.0530
2	22.06	0.0654
3	28.09	0.0350
4	35.02	0.1705
5	37.46	0.0457
6	42.39	0.0332
7	42.96	0.0448
8	46.44	0.0610
9	48.52	0.0013
10	53.03	0.1531
11	53.91	0.0860
12	55.67	0.0619
13	56.58	0.0625
14	59.30	0.3624
15	60.45	0.1097
16	63.24	0.2350
17	65.99	1.2666
18	69.61	0.0546
19	70.93	0.2289
20	74.27	0.0638
21	77.60	0.1127
22	79.40	0.2149
23	80.70	0.2598
24	81.95	0.0262
25	91.56	1.0221
26	93.89	0.0179
27	99.31	0.3214
28	103.96	0.1679
29	109.14	0.8175
30	109.54	1.7520
31	119.40	0.4014
32	125.11	0.4324
33	127.41	1.5661
34	128.62	0.3444
35	137.04	2.1454
36	561.24	68.1034

37	594.19	8.7885
38	1307.33	1.6610
39	2293.93	195.3761

**CO<sub>2</sub>/Ag<sub>13</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.20	0.0305
2	24.71	0.0752
3	31.38	0.0526
4	33.41	0.0483
5	34.60	0.1649
6	40.48	0.0528
7	43.30	0.0288
8	44.64	0.0532
9	45.36	0.0488
10	46.66	0.0030
11	48.81	0.2508
12	51.67	0.0887
13	53.35	0.4414
14	55.81	0.0504
15	57.82	0.2005
16	59.32	0.0290
17	60.32	0.0784
18	63.41	0.1688
19	66.64	0.0052
20	67.70	0.3110
21	70.03	0.0646
22	74.33	0.2496
23	75.75	0.1903
24	79.67	0.0323
25	80.15	0.0186
26	85.40	0.0412
27	86.43	0.0851
28	93.35	0.2634
29	95.74	0.6184
30	103.26	0.0408
31	104.71	0.1611
32	108.39	0.5801
33	111.20	0.5391
34	115.42	2.6445
35	123.43	0.3010
36	125.81	0.3265
37	131.81	0.3954

38	134.63	0.2720
39	572.73	84.6207
40	600.55	9.9023
41	1309.21	0.5636
42	2297.05	357.6131

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**CO<sub>2</sub>/Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.73	0.1344
2	15.21	0.4106
3	22.06	0.2349
4	23.02	0.0206
5	26.18	0.0133
6	32.58	0.0612
7	34.03	0.0574
8	36.77	0.0889
9	41.57	0.1468
10	43.20	0.0167
11	48.16	0.0047
12	49.43	0.0545
13	50.14	0.0537
14	53.96	0.0063
15	57.09	0.1244
16	57.60	0.1395
17	59.22	0.2081
18	61.71	0.3076
19	62.41	0.3773
20	65.12	0.4655
21	65.78	0.1395
22	69.22	0.1193
23	71.73	1.6224
24	74.38	0.5497
25	77.34	0.0286
26	78.50	0.0444
27	83.83	0.1617
28	85.44	0.0216
29	87.27	0.4786
30	94.61	0.0020
31	101.63	0.2192
32	103.91	0.1212
33	106.35	0.1473
34	108.67	0.3699
35	110.68	0.2576

36	113.55	0.1148
37	115.20	0.4830
38	123.39	0.7820
39	127.79	1.2677
40	134.82	0.4768
41	140.07	0.0251
42	556.90	80.1695
43	595.72	7.7518
44	1306.42	1.5170
45	2290.36	168.3377

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**CO<sub>2</sub>/Ag<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.39	0.1507
2	7.10	0.0314
3	24.52	0.0057
4	26.80	0.0002
5	31.17	0.0209
6	32.94	0.0274
7	36.73	0.1272
8	38.71	0.1176
9	40.35	0.2748
10	44.73	0.0619
11	45.87	0.0051
12	47.73	0.1492
13	49.60	0.0051
14	52.60	0.0684
15	54.37	0.0755
16	55.03	0.0318
17	56.65	0.2230
18	59.31	0.0279
19	63.52	0.0014
20	65.49	0.1664
21	66.74	0.0890
22	70.39	0.0635
23	71.76	0.0793
24	72.60	0.0477
25	73.75	0.3102
26	75.53	0.1158
27	76.40	0.0001
28	77.60	0.1609
29	85.21	0.0016
30	89.73	0.0566

31	90.46	0.2226
32	92.01	3.8986
33	98.36	1.2377
34	101.78	0.0559
35	104.01	5.2143
36	105.08	0.0012
37	107.92	0.0090
38	109.58	1.0443
39	111.82	2.8996
40	115.14	0.4685
41	122.93	0.0411
42	123.88	0.0756
43	126.69	2.2453
44	139.93	5.7765
45	619.65	26.3119
46	624.23	26.0569
47	1317.13	2.5771
48	2315.94	1588.1917

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**CO<sub>2</sub>/Ag<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.47	0.0476
2	17.22	0.0342
3	22.16	0.0248
4	25.78	0.0986
5	28.27	0.0541
6	34.15	0.0925
7	35.88	0.0369
8	36.53	0.1076
9	40.47	0.0145
10	42.51	0.1728
11	43.53	0.0386
12	46.43	0.0302
13	47.66	0.1143
14	49.55	0.0431
15	50.89	0.0738
16	51.88	0.1894
17	54.28	0.1761
18	55.92	0.0158
19	56.26	0.2744
20	59.74	0.1030
21	60.09	0.3872
22	61.81	0.1422



23	63.60	0.0181
24	66.48	0.1961
25	69.15	0.0126
26	70.35	0.0282
27	71.64	0.0266
28	72.85	0.1158
29	74.36	0.3097
30	81.10	0.1312
31	83.14	0.0826
32	89.28	0.0776
33	90.83	0.0580
34	91.25	0.0676
35	95.84	1.2942
36	97.30	0.0101
37	101.83	0.0897
38	103.19	0.0354
39	107.95	0.2623
40	110.26	0.4170
41	113.52	0.1970
42	115.01	0.9350
43	118.47	0.2926
44	119.91	0.2273
45	123.70	0.1037
46	128.38	0.0398
47	135.60	0.1081
48	580.91	89.2272
49	602.54	7.8168
50	1310.50	0.1299
51	2299.02	562.1330

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**CO<sub>2</sub>/Ag<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.70	0.0256
2	16.09	0.0692
3	18.15	0.0653
4	20.12	0.4039
5	24.70	0.2997
6	33.28	0.0158
7	34.07	0.5921
8	36.33	0.0289
9	37.73	0.0052
10	39.04	0.2853
11	39.71	0.2301

12	41.77	0.0092
13	43.31	0.0368
14	47.55	0.2948
15	50.99	0.0138
16	53.16	0.7520
17	54.71	0.3183
18	55.65	0.4445
19	56.17	0.0335
20	57.55	0.0243
21	57.98	0.0945
22	62.32	0.4515
23	65.21	0.7572
24	65.86	0.1314
25	66.42	0.1287
26	67.06	0.3158
27	72.14	0.3802
28	73.76	0.1301
29	74.61	0.1112
30	76.96	0.4980
31	79.33	0.2302
32	81.31	0.3345
33	84.36	0.0434
34	85.35	0.1672
35	92.56	0.2136
36	96.84	0.0031
37	97.10	0.0352
38	104.34	0.0720
39	105.66	0.0893
40	106.25	0.0098
41	109.99	0.0110
42	110.41	0.0185
43	110.76	0.0025
44	113.90	0.1201
45	116.45	0.0978
46	119.15	0.0174
47	121.15	0.0265
48	124.16	0.5545
49	126.08	0.5679
50	131.02	0.0081
51	565.41	103.8857
52	599.67	9.5226
53	1308.13	1.5615
54	2292.41	244.6133

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**CO<sub>2</sub>/Ag<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.38	0.0407
2	18.40	0.1087
3	18.81	0.0008
4	19.94	0.1156
5	24.71	0.3702
6	32.78	0.0176
7	33.25	0.6578
8	36.63	0.0400
9	37.18	0.0040
10	40.40	0.0363
11	40.74	0.0047
12	42.54	0.0243
13	43.01	0.0881
14	47.33	0.2617
15	47.41	1.0432
16	50.36	0.4376
17	51.52	0.5455
18	53.17	0.0040
19	54.40	0.1162
20	57.35	0.0080
21	60.04	1.0962
22	60.20	0.0174
23	65.66	1.2043
24	66.60	1.8657
25	67.12	1.3737
26	67.31	0.3189
27	69.05	0.9929
28	69.94	1.2689
29	71.37	0.1977
30	71.61	0.8605
31	73.28	0.0097
32	76.72	0.5322
33	76.79	0.0028
34	83.12	0.1831
35	85.94	0.1016
36	87.95	0.0797
37	93.14	0.0684
38	94.30	0.1578
39	97.17	0.1471
40	100.74	0.3989

41	101.11	0.0342
42	106.24	1.1107
43	108.30	0.0480
44	108.54	0.8320
45	109.09	0.7044
46	111.23	0.1474
47	112.62	0.0668
48	114.86	0.0501
49	115.03	0.0479
50	115.45	0.0598
51	121.17	0.0503
52	123.60	0.0009
53	126.28	0.0005
54	574.65	71.9762
55	605.04	11.1210
56	1308.44	2.0261
57	2291.94	193.5246

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**CO<sub>2</sub>/Ag<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.30	0.1246
2	19.83	0.0503
3	31.23	0.0169
4	33.77	0.0268
5	35.93	0.0251
6	37.51	0.0084
7	38.18	0.0399
8	38.98	0.0386
9	39.75	0.0250
10	41.03	0.0082
11	42.25	0.0638
12	42.44	0.0256
13	43.19	0.0209
14	45.45	0.0245
15	46.91	0.0615
16	47.78	0.0183
17	50.43	0.3157
18	53.24	0.0372
19	54.08	0.0736
20	55.63	0.0356
21	56.45	0.0457
22	57.69	0.3221
23	58.78	0.2368

24	59.69	0.1126
25	61.32	0.2034
26	64.04	0.1307
27	65.33	0.0058
28	66.38	0.0945
29	67.32	0.0254
30	69.92	0.0633
31	71.28	0.1635
32	72.51	0.0682
33	73.94	0.0849
34	75.18	0.1242
35	76.54	0.1728
36	78.43	0.0582
37	79.95	0.0167
38	80.33	0.0069
39	83.31	0.0692
40	90.03	0.8532
41	92.58	0.1649
42	95.44	0.4381
43	97.44	0.0174
44	98.65	0.8744
45	99.78	0.4243
46	104.93	0.1629
47	105.58	0.2597
48	107.17	0.2463
49	110.68	0.2749
50	118.42	0.0958
51	121.72	0.2638
52	133.66	0.1296
53	135.65	0.2726
54	136.40	0.6253
55	137.94	0.0505
56	142.89	0.1201
57	568.27	93.3688
58	588.74	4.9602
59	1306.93	1.8519
60	2293.18	341.8146

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**CO<sub>2</sub>/Ag<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	0.41	0.0372
2	12.78	0.1241
3	22.15	0.0034

4	33.10	0.0301
5	33.46	0.0519
6	35.76	0.0781
7	37.74	0.0641
8	38.66	0.0298
9	40.71	0.1014
10	41.89	0.1378
11	44.00	0.0043
12	45.37	0.0657
13	45.93	0.0498
14	47.67	0.0630
15	48.15	0.0938
16	49.05	0.0949
17	51.01	0.2256
18	53.42	0.1239
19	53.93	0.0892
20	55.49	0.0423
21	55.85	0.1221
22	56.32	0.0175
23	59.13	0.0527
24	59.63	0.0875
25	61.20	0.0677
26	62.63	0.0145
27	63.54	0.0155
28	64.50	0.0543
29	65.51	0.0045
30	67.78	0.0448
31	70.57	0.0080
32	71.47	0.0105
33	73.74	0.0105
34	77.17	0.0703
35	78.07	0.0147
36	78.43	0.0569
37	79.69	0.0749
38	80.63	0.0095
39	81.71	0.0309
40	83.74	0.0153
41	85.12	0.0030
42	85.54	0.0119
43	91.22	0.0236
44	93.76	0.1282
45	96.38	0.2049
46	97.36	0.2079

47	103.33	0.0454
48	103.99	0.0331
49	107.99	0.0766
50	115.62	1.3860
51	118.17	0.0547
52	121.71	0.8084
53	127.62	1.6203
54	131.16	0.5719
55	132.89	0.6832
56	134.14	0.3562
57	135.90	0.4552
58	140.82	0.0358
59	144.25	1.6960
60	587.83	74.1479
61	604.81	9.5770
62	1311.22	0.3668
63	2301.23	566.6033

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**CO<sub>2</sub>/Ag<sub>21</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.52	0.0259
2	23.26	0.0702
3	28.68	0.0557
4	31.49	0.0929
5	31.76	0.0570
6	34.74	0.0224
7	35.60	0.1647
8	36.68	0.0500
9	39.77	0.0311
10	40.86	0.0476
11	41.09	0.0214
12	44.25	0.0539
13	44.43	0.2307
14	46.05	0.1054
15	46.53	0.0783
16	47.49	0.0342
17	48.26	0.0615
18	49.01	0.0660
19	50.48	0.0291
20	51.46	0.0186
21	52.94	0.0159
22	54.91	0.1970
23	55.44	0.0490

24	56.04	0.0175
25	56.09	0.0123
26	57.91	0.2617
27	58.48	0.1417
28	59.85	0.0212
29	62.25	0.1211
30	62.88	0.0683
31	64.96	0.0675
32	68.85	0.1798
33	70.07	0.0201
34	70.68	0.1144
35	72.21	0.1517
36	72.51	0.1164
37	73.13	0.0773
38	76.25	0.0063
39	78.58	0.0247
40	83.97	0.0768
41	86.67	0.7384
42	87.53	0.3335
43	88.58	0.0178
44	90.52	0.3429
45	92.64	0.3469
46	95.44	0.1428
47	96.02	0.0313
48	98.29	0.1042
49	99.89	0.5816
50	101.68	0.2871
51	105.42	0.4036
52	106.01	0.0113
53	107.62	1.5598
54	109.16	0.1499
55	109.62	0.4343
56	119.85	0.7014
57	121.82	0.0834
58	122.17	0.1684
59	123.84	0.0870
60	125.61	0.0131
61	128.51	0.2912
62	129.17	0.1089
63	575.08	95.6744
64	598.74	5.6585
65	1307.41	0.6948
66	2292.70	372.8659



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**CO<sub>2</sub>/Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.94	0.1144
2	20.06	0.0526
3	22.52	0.0037
4	24.67	0.1340
5	30.45	0.0148
6	30.96	0.0122
7	34.70	0.1615
8	38.82	0.1363
9	39.47	0.0300
10	39.77	0.0539
11	41.15	0.0274
12	42.73	0.0763
13	43.87	0.0203
14	44.37	0.1368
15	45.58	0.0343
16	47.35	0.0301
17	47.42	0.1130
18	49.15	0.0402
19	50.24	0.0968
20	50.89	0.0839
21	51.49	0.0220
22	52.34	0.0324
23	54.19	0.2611
24	55.05	0.1245
25	55.96	0.5929
26	56.59	0.0608
27	57.45	0.2270
28	59.43	0.4044
29	61.03	0.1744
30	62.06	0.0027
31	63.34	0.4613
32	66.07	0.1335
33	66.37	0.1979
34	68.64	0.2761
35	69.80	0.1865
36	71.12	0.2120
37	71.84	0.4048
38	72.78	0.0405
39	76.01	0.3958
40	77.02	0.2241

41	77.96	0.0174
42	81.08	0.2213
43	82.00	0.0558
44	82.67	0.4224
45	84.97	0.0633
46	87.01	0.1432
47	88.46	0.1318
48	89.78	0.8238
49	91.52	0.4541
50	92.90	0.8381
51	96.50	0.7551
52	98.67	0.0632
53	102.60	0.0898
54	105.71	0.1202
55	108.36	0.2561
56	111.24	0.7333
57	118.95	0.2460
58	120.82	0.6557
59	125.06	0.0764
60	126.42	0.0381
61	128.97	0.3098
62	130.81	0.1020
63	137.76	0.1142
64	142.57	0.0415
65	158.07	0.3894
66	538.51	54.3487
67	583.48	6.9059
68	1304.28	9.4827
69	2287.09	141.9427

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**NO/Ag<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	217.44	3.6792
2	393.81	11.3768
3	1572.48	1349.7392

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**NO/Ag<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.16	0.1066
2	124.03	0.7273
3	159.42	0.8601
4	160.55	1.8058
5	267.80	10.8399
6	1773.80	677.9785

NO/Ag <sub>3</sub>		
Mode	Frequency	Infrared
1	19.29	2.1541
2	73.96	4.6111
3	90.32	2.9790
4	129.92	1.8548
5	135.55	0.1106
6	136.24	0.0040
7	252.63	32.4370
8	408.90	32.1422
9	1587.00	318.4028

NO/Ag <sub>4</sub>		
Mode	Frequency	Infrared
1	26.51	0.3817
2	29.34	0.0718
3	45.85	5.8535
4	70.22	0.4351
5	76.62	0.4489
6	92.22	0.4116
7	124.01	2.9913
8	133.34	2.7756
9	151.89	8.1497
10	208.58	12.2968
11	263.99	21.2186
12	1950.07	677.1358

NO/Ag <sub>5</sub>		
Mode	Frequency	Infrared
1	15.03	0.1311
2	18.95	0.1517
3	43.62	1.6893
4	54.02	0.7441
5	70.88	1.0194
6	86.79	2.5148
7	87.46	0.4394
8	94.90	1.2033
9	106.91	0.0756
10	136.53	0.9039
11	136.86	2.7104
12	197.22	2.9120
13	251.01	115.9599
14	378.51	37.2047
15	1523.65	558.3025

NO/Ag <sub>6</sub>		
Mode	Frequency	Infrared
1	18.00	0.1018
2	19.15	0.0090
3	24.13	0.0774
4	27.73	0.1465
5	31.52	0.2433
6	57.73	0.1951
7	58.38	0.0319
8	70.80	0.2371
9	72.42	0.4762
10	74.73	0.8371
11	77.65	0.5935
12	100.84	0.0037
13	109.66	0.0206
14	118.40	0.0151
15	153.47	6.5138
16	153.86	5.5720
17	157.00	4.1008
18	1795.81	504.4673

NO/Ag <sub>7</sub>		
Mode	Frequency	Infrared
1	27.30	1.4404
2	35.32	0.1188
3	39.65	0.1474
4	48.20	0.5365
5	50.28	0.2248
6	59.28	0.0052
7	63.36	0.0297
8	64.21	0.0288
9	65.81	1.1093
10	73.35	1.6068
11	82.23	0.4776
12	90.07	0.0597
13	91.65	0.6410
14	115.90	0.0467
15	125.46	0.3150
16	132.76	0.5409
17	147.77	1.0069
18	193.12	0.2707
19	255.07	18.7444
20	408.76	6.6777

21

1561.04

399.8978

NO/Ag<sub>8</sub>

Mode	Frequency	Infrared
1	22.62	0.0665
2	26.47	0.0197
3	41.15	0.0030
4	43.61	0.1720
5	47.64	0.0803
6	55.32	0.2700
7	56.62	0.2144
8	57.59	0.0067
9	62.27	0.0691
10	63.86	0.0040
11	65.70	0.0119
12	73.01	0.0305
13	87.05	0.0771
14	90.53	0.0655
15	90.68	0.1124
16	102.39	0.0082
17	109.92	0.0286
18	116.66	0.0071
19	118.61	0.0103
20	126.08	0.1032
21	128.72	0.0022
22	157.09	1.0908
23	219.24	1.5831
24	1791.74	504.8500

NO/Ag<sub>9</sub>

Mode	Frequency	Infrared
1	17.94	0.0167
2	26.44	0.0795
3	30.02	1.4205
4	33.23	0.6069
5	38.63	0.2380
6	46.80	0.2988
7	49.26	0.2653
8	54.75	0.4630
9	63.03	1.0503
10	65.70	0.3761
11	71.71	0.5899
12	76.14	0.1893
13	81.21	0.2639

14	83.15	0.1252
15	86.03	0.4002
16	90.05	0.4111
17	95.16	0.7892
18	99.40	0.3849
19	113.19	0.0160
20	120.60	0.1840
21	122.79	0.2324
22	145.91	0.3564
23	162.83	1.4782
24	197.46	1.0534
25	261.95	31.9088
26	414.60	3.4133
27	1570.03	352.6897

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**NO/Ag<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.85	7.4018
2	10.42	0.3428
3	31.50	3.6477
4	32.68	0.2088
5	44.22	0.2116
6	48.66	0.3933
7	51.07	1.8718
8	53.04	6.0886
9	55.75	0.5243
10	61.49	2.2110
11	65.52	0.2550
12	69.30	0.2782
13	71.88	0.2753
14	77.50	0.8113
15	81.48	1.0685
16	84.84	0.0562
17	88.12	0.5564
18	91.85	0.5208
19	99.83	3.7966
20	105.25	3.0679
21	111.02	0.6298
22	114.50	0.5503
23	117.63	0.7500
24	119.50	0.2890
25	131.47	2.6341
26	143.29	4.0687

27	155.71	5.9673
28	244.47	9.5589
29	280.92	6.2134
30	1128.01	1691.5506

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**NO/Ag<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.29	0.0392
2	27.39	0.9962
3	31.27	0.0719
4	35.66	0.3520
5	37.79	0.3133
6	42.19	0.1282
7	43.93	0.1639
8	49.21	0.1454
9	51.25	0.4093
10	53.77	0.1052
11	58.63	0.1397
12	60.57	0.2038
13	65.70	0.1106
14	67.69	0.3917
15	69.64	1.2724
16	72.48	0.2547
17	77.05	0.2308
18	81.86	0.6535
19	84.14	0.1706
20	92.84	0.1492
21	97.10	0.2085
22	102.22	1.2909
23	105.68	0.1925
24	113.49	0.0200
25	116.88	0.0837
26	121.03	0.7687
27	122.40	1.4930
28	132.62	0.1017
29	159.85	1.8894
30	201.30	2.9206
31	251.48	28.2900
32	406.50	3.2151
33	1551.51	374.8526

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**NO/Ag<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.18	0.1703

2	24.95	0.1281
3	31.46	0.2029
4	35.81	0.2139
5	36.58	0.0959
6	39.93	0.0324
7	42.42	0.0296
8	47.37	0.1047
9	47.93	0.2534
10	49.64	0.6299
11	53.85	0.1110
12	55.83	0.3899
13	57.99	0.1499
14	63.31	0.3237
15	66.02	0.0670
16	73.07	0.2209
17	75.78	0.5541
18	76.82	0.2604
19	79.96	0.1258
20	82.20	0.4679
21	84.92	0.1883
22	89.27	1.4245
23	95.64	0.4842
24	100.87	0.1194
25	106.46	1.1331
26	108.80	0.3925
27	112.48	0.4602
28	117.22	0.6748
29	122.21	0.7103
30	126.64	1.6138
31	129.03	0.6336
32	136.62	1.8729
33	182.24	7.8101
34	226.39	12.0390
35	262.42	16.9997
36	1259.29	5.0538

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**NO/Ag<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	26.37	0.0972
2	32.29	0.2474
3	32.57	0.2475
4	36.42	1.6890
5	41.82	0.3325



6	42.80	0.1012
7	44.48	0.0713
8	45.69	0.0537
9	48.32	0.4226
10	49.77	0.7657
11	51.86	0.1653
12	56.08	0.3088
13	57.41	0.6714
14	60.98	0.3728
15	63.93	0.3596
16	64.83	0.4678
17	69.45	0.0751
18	71.26	0.2055
19	73.02	0.0597
20	74.04	0.4092
21	77.38	0.1023
22	80.61	0.5390
23	81.64	0.5834
24	86.16	1.0087
25	91.69	0.1473
26	96.94	0.0902
27	98.56	0.3185
28	105.75	0.0755
29	106.40	0.2303
30	110.07	1.2034
31	121.09	0.2616
32	125.79	0.0207
33	127.50	0.0527
34	132.05	0.1777
35	136.29	0.1611
36	146.88	0.0376
37	206.99	3.8153
38	307.97	3.8027
39	1277.40	687.4888

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**NO/Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.15	0.1631
2	19.33	0.4708
3	21.14	0.0184
4	23.31	0.0648
5	26.00	0.0103
6	31.86	0.0363

7	36.65	0.1189
8	41.56	0.0969
9	42.83	0.0275
10	48.51	0.0082
11	50.08	0.0573
12	52.29	0.1293
13	55.38	0.0117
14	57.70	0.2836
15	59.23	0.2661
16	59.55	0.2228
17	60.90	0.0776
18	64.16	0.0741
19	64.93	0.3555
20	67.33	0.2067
21	71.96	0.1048
22	73.51	0.2516
23	76.51	0.0217
24	78.96	0.0631
25	82.09	0.1278
26	84.71	0.1114
27	85.73	0.1438
28	95.98	0.0294
29	99.30	0.5656
30	101.35	0.0300
31	103.81	0.2213
32	108.63	0.2971
33	110.41	0.0691
34	112.66	0.0935
35	115.67	0.5206
36	121.12	2.1658
37	126.28	1.2388
38	133.04	1.2958
39	137.77	2.3596
40	147.61	11.6572
41	191.27	17.7686
42	1679.31	4512.6196

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NO/Ag<sub>15</sub>

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Mode	Frequency	Infrared
1	7.67	3.7436
2	23.36	0.0511
3	28.59	0.1247
4	29.96	0.1902

5	31.11	0.0025
6	31.23	0.0140
7	33.55	0.0009
8	38.86	0.0040
9	46.19	0.0447
10	50.86	0.8499
11	51.87	1.3261
12	53.05	0.5497
13	54.96	0.0707
14	57.47	0.0692
15	59.24	0.3598
16	60.74	0.0405
17	61.75	0.1765
18	64.99	0.0075
19	65.51	0.2862
20	68.68	0.0376
21	68.93	0.0094
22	74.23	0.1756
23	78.13	0.9677
24	79.87	0.2112
25	80.92	0.0917
26	85.36	0.0554
27	85.61	0.0131
28	96.98	0.0104
29	98.38	0.4945
30	100.98	0.0306
31	102.30	0.0405
32	107.38	0.1103
33	109.13	0.2731
34	111.54	0.0014
35	112.59	0.0758
36	116.36	0.1726
37	117.23	0.3651
38	121.04	0.9550
39	122.15	1.2901
40	123.20	0.1091
41	128.10	0.0244
42	142.87	0.6137
43	229.46	24.2403
44	312.11	1.6889
45	1271.23	238.2178

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**NO/Ag<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.70	0.0132
2	23.55	0.2123
3	28.96	0.0451
4	31.09	0.1511
5	32.96	0.3080
6	33.14	0.0839
7	36.73	0.1359
8	39.45	0.0336
9	42.74	0.1271
10	44.56	0.0105
11	47.16	0.1025
12	48.85	0.1395
13	53.08	0.0439
14	53.75	0.1197
15	54.73	0.0597
16	58.59	0.0483
17	60.38	0.3542
18	61.04	0.1399
19	61.62	0.3804
20	64.69	0.2007
21	65.18	0.3034
22	68.82	0.3949
23	70.57	0.3172
24	72.63	0.6410
25	74.41	0.3010
26	78.96	0.2045
27	81.57	0.1668
28	84.07	0.2185
29	85.79	0.3280
30	89.06	0.0597
31	92.94	0.1409
32	97.38	0.4212
33	98.72	0.0948
34	102.42	0.4270
35	103.58	0.1131
36	107.55	0.1447
37	109.08	0.3820
38	112.13	0.3952
39	113.37	0.0991
40	115.06	0.2064
41	118.74	0.2731
42	125.54	0.1694

43	130.55	0.3317
44	132.60	0.0599
45	210.80	22.4934
46	221.14	8.9390
47	248.53	2.0551
48	1505.86	149.1373

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**NO/Ag<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.55	0.2317
2	24.72	0.4728
3	28.35	0.2406
4	29.52	0.1789
5	31.94	0.5385
6	33.47	0.3919
7	35.26	0.3671
8	35.97	0.5776
9	40.16	0.0472
10	41.76	0.1612
11	42.80	0.2423
12	44.39	0.2279
13	47.11	0.2160
14	48.91	0.0618
15	50.45	0.0724
16	53.12	0.1032
17	57.47	0.1195
18	58.23	0.0582
19	59.83	0.1384
20	60.23	0.1821
21	62.84	0.0416
22	65.20	0.4335
23	67.16	0.4336
24	68.85	0.3752
25	70.49	0.1452
26	73.92	0.5974
27	75.04	0.2806
28	76.11	0.0509
29	77.96	0.4780
30	83.07	0.2461
31	87.32	0.2247
32	88.76	0.0062
33	92.27	0.5032
34	93.69	0.0255

35	96.89	0.2027
36	98.34	0.1184
37	102.96	0.1544
38	106.32	0.0636
39	114.99	0.1672
40	117.17	0.1606
41	118.98	0.1594
42	120.55	0.4872
43	124.72	1.1964
44	126.57	0.4353
45	136.83	0.7737
46	139.83	0.4120
47	160.90	1.7097
48	199.92	0.9262
49	242.35	20.2991
50	401.13	1.7747
51	1531.61	437.6424

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**NO/Ag<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.19	0.0061
2	16.12	0.0175
3	21.85	0.3847
4	23.42	0.0791
5	24.90	0.1520
6	27.53	0.0841
7	29.31	0.0085
8	38.04	0.0215
9	39.63	0.0470
10	40.77	0.1461
11	43.20	0.0485
12	46.20	0.2978
13	47.49	0.0220
14	48.64	0.0699
15	49.41	0.0189
16	51.12	0.0659
17	52.04	0.2506
18	54.61	0.3723
19	58.13	0.1480
20	60.24	0.1153
21	60.92	0.3044
22	61.48	1.4328
23	63.36	0.0087

24	64.40	0.0957
25	65.93	1.0321
26	71.92	0.0928
27	72.65	0.0950
28	74.47	0.5531
29	75.13	0.9379
30	77.22	0.0430
31	78.50	0.0436
32	81.04	1.8494
33	81.95	0.1342
34	85.59	0.3064
35	87.14	0.2955
36	92.34	0.0529
37	93.92	0.0726
38	94.82	0.0040
39	97.03	0.1369
40	105.16	0.1798
41	106.43	1.1544
42	108.40	0.4486
43	109.78	0.1957
44	109.94	0.3895
45	110.75	0.2541
46	111.66	0.0202
47	112.60	0.4717
48	113.67	0.5145
49	114.99	0.1331
50	119.21	0.0641
51	121.80	0.0177
52	124.70	0.0162
53	153.59	0.1812
54	1751.54	1807.4583

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**NO/Ag<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.02	1.1096
2	26.36	0.1254
3	30.46	0.0716
4	31.88	0.0834
5	33.96	0.0224
6	35.43	0.0764
7	39.00	0.0746
8	39.41	0.0175
9	40.19	0.0403

10	42.96	0.0464
11	44.42	0.4958
12	45.47	0.5048
13	46.90	0.0628
14	49.04	0.0893
15	49.31	0.0230
16	52.07	0.2615
17	52.94	0.1267
18	53.84	0.0392
19	56.40	0.0323
20	57.29	0.1416
21	58.03	0.0631
22	60.26	0.6582
23	61.61	0.2871
24	63.88	0.0369
25	65.36	0.0508
26	67.74	0.2753
27	69.79	0.1106
28	72.30	0.0500
29	75.08	0.1217
30	76.75	0.2251
31	78.32	0.1159
32	78.65	0.2500
33	80.04	0.0448
34	82.57	0.1710
35	84.46	0.1909
36	85.61	0.3813
37	87.94	0.0625
38	90.28	0.1144
39	93.32	0.0778
40	94.40	0.1626
41	95.78	0.1318
42	99.99	0.0405
43	102.32	0.1359
44	104.84	0.0951
45	109.31	0.0110
46	115.08	0.1069
47	121.32	0.4332
48	125.64	0.0880
49	129.96	0.6790
50	141.28	0.0238
51	145.56	0.1001
52	146.73	1.0333



53	156.05	0.1196
54	187.91	0.3965
55	240.87	23.2692
56	407.24	2.7395
57	1543.97	451.1209

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**NO/Ag<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.15	0.1405
2	21.55	0.0311
3	22.77	0.0131
4	30.63	0.0787
5	32.03	0.0895
6	39.89	0.0771
7	41.46	0.0237
8	42.06	0.0111
9	43.44	0.0119
10	44.29	0.0744
11	45.29	0.0292
12	49.28	0.0626
13	50.00	0.0783
14	52.42	0.0176
15	53.69	0.1298
16	54.24	0.1794
17	55.38	0.1615
18	56.90	0.0528
19	58.05	0.0651
20	59.42	0.0211
21	60.31	0.0407
22	61.75	0.0161
23	63.82	0.0291
24	63.91	0.0241
25	64.71	0.0336
26	66.23	0.0538
27	69.81	0.0111
28	71.12	0.0528
29	71.52	0.0635
30	72.22	0.0590
31	73.19	0.0074
32	73.49	0.0396
33	76.84	0.0151
34	79.11	0.0463
35	79.48	0.0065

36	81.42	0.2051
37	84.22	0.2339
38	87.52	0.0428
39	87.72	0.0208
40	91.26	0.0141
41	93.02	0.1115
42	93.52	0.0386
43	94.59	0.0277
44	97.07	0.0301
45	106.58	0.0443
46	107.35	0.0100
47	107.97	0.0994
48	109.53	0.0623
49	109.99	0.1320
50	111.47	0.0273
51	114.00	0.0863
52	115.27	0.1233
53	117.60	0.1716
54	125.48	0.0334
55	127.37	0.0856
56	128.05	0.2339
57	128.94	0.5462
58	129.29	0.0819
59	135.41	0.2052
60	1817.62	722.8668

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**NO/Ag<sub>21</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.43	3.3727
2	27.84	0.1139
3	30.24	0.2456
4	31.05	0.1792
5	32.19	0.1489
6	36.13	0.1149
7	37.33	0.0732
8	39.80	0.1786
9	40.86	0.0776
10	41.78	0.2197
11	43.07	0.0771
12	43.73	0.1509
13	45.91	0.1787
14	47.54	0.2468
15	49.08	0.2222

16	49.46	0.0770
17	51.15	0.0390
18	51.78	0.3659
19	52.52	0.3189
20	53.59	0.1875
21	54.99	0.0905
22	57.69	0.0675
23	57.96	0.0560
24	60.59	0.1620
25	61.49	0.3802
26	62.34	0.1939
27	63.69	0.1026
28	65.49	0.5255
29	66.24	0.3520
30	67.56	0.1549
31	70.15	0.1002
32	70.54	0.0490
33	72.70	0.0610
34	75.16	0.0399
35	78.24	0.0291
36	79.46	0.1380
37	81.11	0.1648
38	83.58	0.4905
39	84.80	0.0440
40	88.85	0.1133
41	91.45	0.1186
42	92.20	0.0901
43	95.43	0.0407
44	96.86	0.1731
45	99.91	0.0384
46	101.24	0.2692
47	103.11	0.0267
48	103.51	0.0230
49	105.11	0.0090
50	108.69	0.1747
51	111.65	0.3255
52	115.54	0.3557
53	119.51	0.5945
54	122.45	0.2539
55	124.78	0.5945
56	125.28	0.3793
57	127.03	0.2286
58	131.66	0.2017

59	137.57	0.7971
60	141.80	0.1194
61	226.42	24.3940
62	327.10	0.8896
63	1276.72	106.3218

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**NO/Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.84	0.1145
2	28.86	0.0480
3	29.06	0.5422
4	32.41	0.0532
5	36.22	0.1413
6	36.33	1.1277
7	39.57	0.1488
8	40.01	0.0828
9	41.28	0.0258
10	43.88	0.0193
11	45.44	0.3898
12	46.15	0.1955
13	47.24	0.1136
14	47.81	0.1172
15	49.29	0.0072
16	50.90	0.0933
17	51.52	0.0783
18	52.68	0.0626
19	53.38	0.5067
20	53.94	0.0292
21	55.31	0.1208
22	56.32	0.0241
23	56.70	0.0838
24	58.53	0.0275
25	58.93	0.0362
26	60.82	0.0081
27	62.32	0.5193
28	63.76	0.0580
29	64.61	0.1440
30	65.78	0.0925
31	67.72	0.0302
32	69.41	0.2312
33	70.67	0.0360
34	72.60	0.0516
35	74.58	0.7359

36	75.13	0.0433
37	76.31	0.0211
38	78.14	0.0111
39	79.68	0.1066
40	80.30	0.2305
41	80.96	0.2771
42	82.04	0.0277
43	82.85	0.0641
44	84.63	0.1407
45	87.53	0.0244
46	90.39	0.0372
47	92.31	0.0509
48	93.31	0.0341
49	100.83	0.0617
50	101.23	0.2720
51	105.41	0.0074
52	107.68	0.0855
53	118.28	0.7245
54	121.02	0.4481
55	122.97	0.0313
56	124.80	0.1789
57	132.22	0.1048
58	133.41	0.0975
59	138.72	0.0150
60	140.66	0.2233
61	152.03	0.1424
62	163.74	7.0347
63	165.14	1.2880
64	247.32	9.9717
65	374.81	8.7225
66	1436.23	308.4662

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**NO<sub>2</sub>/Ag<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	187.19	0.4049
2	285.88	16.7591
3	321.91	11.2058
4	822.05	0.5348
5	1231.91	497.5524
6	1261.82	3.8422

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**NO<sub>2</sub>/Ag<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.94	2.2706

2	22.71	2.8611
3	97.97	0.4710
4	165.93	0.4554
5	277.26	27.1375
6	304.82	5.5086
7	812.49	0.0231
8	1232.29	415.9710
9	1263.11	24.4978

**NO<sub>2</sub>/Ag<sub>3</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	41.74	3.2216
2	54.50	7.6503
3	76.07	0.0004
4	94.00	1.8854
5	110.38	0.7902
6	148.57	1.0188
7	213.02	0.4874
8	283.69	55.2172
9	284.68	3.5548
10	767.21	10.7722
11	1245.66	332.2829
12	1291.38	4.4520

**NO<sub>2</sub>/Ag<sub>4</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.51	0.0179
2	44.16	2.6286
3	62.73	4.7729
4	70.05	0.0251
5	70.15	0.3377
6	73.47	0.3447
7	95.13	0.0323
8	126.11	0.1141
9	127.32	0.1358
10	237.81	0.9648
11	289.66	33.1991
12	295.66	22.0033
13	774.14	6.4175
14	1257.96	291.4038
15	1294.50	15.0902

**NO<sub>2</sub>/Ag<sub>5</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.88	0.0001

2	27.16	0.0740
3	45.37	2.5514
4	51.18	0.0332
5	58.43	4.1383
6	59.61	0.0036
7	67.12	0.1274
8	76.80	0.0768
9	109.34	0.3423
10	112.28	1.2706
11	130.20	0.0038
12	152.72	3.7768
13	248.23	1.4346
14	299.09	53.3814
15	301.27	2.0307
16	777.53	4.2794
17	1269.06	419.3897
18	1299.35	2.7333

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**NO<sub>2</sub>/Ag<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	33.71	3.2024
2	34.47	0.0116
3	40.98	0.0002
4	47.52	0.0464
5	62.89	2.7110
6	64.62	0.0005
7	66.15	0.0002
8	70.26	1.1901
9	73.22	0.0144
10	81.79	0.0001
11	89.67	0.3785
12	90.64	0.4882
13	105.88	0.5995
14	132.27	0.0005
15	135.69	0.0352
16	256.70	2.5907
17	302.69	44.2050
18	307.11	0.1678
19	778.24	4.0942
20	1265.60	302.7450
21	1293.40	0.1598

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**NO<sub>2</sub>/Ag<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
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1	19.31	3.2827
2	39.17	0.2270
3	41.72	0.0484
4	50.67	0.5450
5	51.68	0.0542
6	65.84	1.5530
7	66.39	0.0945
8	68.40	0.0574
9	69.55	0.1072
10	70.00	0.0022
11	77.24	0.7499
12	80.90	0.5360
13	92.33	0.1247
14	92.40	0.1254
15	111.88	0.6727
16	130.16	0.1054
17	132.03	0.3752
18	143.72	2.8930
19	186.29	0.0004
20	278.81	59.1484
21	298.70	1.1479
22	782.04	30.5366
23	1211.68	132.5791
24	1483.89	303.6084

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**NO<sub>2</sub>/Ag<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	27.67	0.2284
2	29.53	0.8909
3	31.52	1.4231
4	36.62	0.4848
5	51.10	1.2548
6	53.78	0.4041
7	57.60	0.8025
8	60.02	0.1024
9	62.02	0.0652
10	66.82	0.1774
11	68.02	0.6007
12	70.22	0.0243
13	74.55	0.0214
14	86.20	0.1887
15	86.43	0.3296
16	95.37	0.3344



17	100.01	0.0778
18	108.81	0.0538
19	114.40	0.2669
20	119.23	0.0451
21	123.52	0.0605
22	226.41	0.5073
23	276.08	31.3676
24	290.98	24.3518
25	771.06	4.4845
26	1252.68	216.2719
27	1288.90	1.5923

**NO<sub>2</sub>/Ag<sub>9</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.01	1.1505
2	30.36	0.2049
3	31.62	0.0920
4	35.51	0.3924
5	38.33	0.4894
6	44.79	0.3124
7	48.77	0.0291
8	49.04	0.1967
9	54.82	0.3707
10	57.59	0.8700
11	63.35	0.1207
12	66.92	0.5729
13	73.14	0.5521
14	79.39	0.8018
15	84.04	0.2960
16	87.72	0.4903
17	89.48	0.9010
18	94.34	0.1039
19	112.67	0.0499
20	115.06	0.9008
21	126.53	1.1138
22	127.60	0.0184
23	134.59	0.4101
24	137.16	0.5056
25	186.71	1.2134
26	239.65	45.5060
27	270.19	4.1547
28	746.18	26.8476
29	1058.83	189.8010

30

1544.58

267.7848

**NO<sub>2</sub>/Ag<sub>10</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.48	0.0683
2	26.07	1.2954
3	27.71	1.1263
4	32.32	0.2932
5	35.76	0.1982
6	40.87	0.5643
7	51.45	0.1870
8	55.34	0.0621
9	55.60	0.1236
10	58.45	0.1878
11	62.04	1.5129
12	64.33	0.4343
13	66.79	0.0203
14	71.27	1.5507
15	71.69	0.5151
16	73.18	0.0633
17	79.11	0.0920
18	80.02	0.2455
19	88.17	0.1580
20	94.42	0.0391
21	97.51	0.0400
22	100.72	0.1952
23	110.98	0.0824
24	115.46	0.1470
25	121.19	0.8085
26	123.38	0.3658
27	128.70	0.8523
28	219.26	0.3631
29	280.06	46.6460
30	289.40	18.8570
31	772.03	7.5562
32	1250.65	214.5645
33	1292.83	5.0452

**NO<sub>2</sub>/Ag<sub>11</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.94	0.1233
2	28.42	0.1115
3	30.81	0.9750
4	34.34	0.1897

5	37.72	0.0851
6	40.22	0.1368
7	44.10	1.5512
8	48.01	0.1222
9	49.33	0.5139
10	54.83	0.3121
11	56.61	0.1984
12	58.76	0.6286
13	62.00	0.2101
14	68.77	0.8297
15	71.04	0.7214
16	73.73	0.3425
17	78.53	0.9019
18	79.98	0.7558
19	85.55	0.4705
20	89.43	0.5548
21	92.87	0.2062
22	97.39	0.5229
23	106.54	0.1540
24	109.04	0.5261
25	113.30	1.4041
26	115.77	0.3875
27	125.70	1.6254
28	129.00	0.9276
29	133.91	0.7937
30	140.92	0.7084
31	156.90	3.5345
32	236.95	73.3587
33	263.24	1.6877
34	750.80	35.6562
35	1091.43	222.1610
36	1533.40	301.8156

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**NO<sub>2</sub>/Ag<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	24.31	2.1088
2	26.30	0.6186
3	32.23	0.2503
4	35.20	0.3281
5	39.26	0.0384
6	40.89	0.1725
7	48.96	0.1097
8	50.06	0.0580

9	51.38	0.0824
10	53.82	0.1732
11	56.57	0.1627
12	59.74	0.0586
13	61.65	0.3697
14	64.37	0.0058
15	65.41	0.7888
16	66.54	0.6182
17	72.75	0.0443
18	73.23	0.0251
19	75.75	0.6494
20	80.04	0.3513
21	80.69	0.5088
22	83.15	0.1543
23	88.68	0.2332
24	91.86	0.0239
25	96.73	0.1634
26	101.21	0.0328
27	107.04	0.0336
28	108.37	0.0740
29	114.06	0.0292
30	125.41	0.1026
31	132.16	0.0647
32	133.79	0.3652
33	152.59	0.8310
34	181.10	2.1423
35	277.70	21.3620
36	282.03	54.2252
37	790.07	27.7621
38	1206.74	121.6966
39	1487.32	260.8079

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**NO<sub>2</sub>/Ag<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.33	2.4534
2	26.24	0.5022
3	31.49	0.1809
4	33.30	0.1564
5	39.92	0.1462
6	42.03	0.0682
7	43.60	0.0934
8	45.40	0.0454
9	49.07	0.1856

10	51.04	0.3613
11	51.51	0.0205
12	54.14	0.1578
13	57.78	0.7809
14	62.10	0.5108
15	63.06	0.1982
16	66.21	1.0187
17	69.88	0.0639
18	71.48	0.3359
19	73.37	0.0780
20	76.02	0.4551
21	77.59	0.2502
22	79.19	0.1774
23	84.20	0.2532
24	86.79	0.1962
25	89.20	0.1072
26	94.69	0.2654
27	98.00	0.7216
28	100.94	0.0737
29	103.95	0.1867
30	108.61	0.4195
31	112.70	0.4415
32	122.44	0.9460
33	128.29	0.2113
34	133.49	0.4117
35	135.52	0.0437
36	151.54	1.2363
37	173.81	4.4521
38	265.73	4.8442
39	284.88	70.7433
40	789.24	26.5136
41	1203.07	131.8849
42	1486.80	250.5317

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**NO<sub>2</sub>/Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	25.99	0.1279
2	27.41	0.1916
3	33.49	0.1022
4	36.61	0.0717
5	41.20	0.0261
6	43.08	0.2963
7	45.31	0.3059

8	48.01	0.0621
9	49.61	0.4551
10	51.65	0.0342
11	55.30	0.9735
12	57.20	0.4349
13	58.06	0.4092
14	60.51	0.2497
15	61.68	0.5459
16	63.06	0.0478
17	64.42	0.2021
18	67.23	0.0491
19	69.75	0.2640
20	70.67	0.1530
21	73.34	0.2246
22	74.84	0.5352
23	76.53	0.0770
24	80.75	0.2261
25	81.23	1.4217
26	86.06	0.0840
27	89.93	0.1403
28	92.69	0.3747
29	96.06	0.0650
30	98.43	0.6196
31	102.43	0.2329
32	105.98	0.1004
33	106.75	3.0291
34	112.13	0.3973
35	119.85	0.2758
36	123.60	0.1329
37	128.14	0.1898
38	133.45	0.1702
39	136.49	0.2057
40	184.90	23.0164
41	195.92	1.1546
42	232.94	15.3511
43	775.22	3.4355
44	1117.42	271.9609
45	1354.01	68.6912

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**NO<sub>2</sub>/Ag<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.39	2.5342
2	24.00	0.2871

3	27.83	0.0295
4	30.48	0.0991
5	31.31	0.2859
6	33.06	0.0333
7	34.00	0.3542
8	38.75	0.1228
9	47.54	0.0550
10	48.20	0.0776
11	50.12	0.0241
12	53.15	0.0394
13	55.51	0.5146
14	57.05	0.2153
15	58.26	0.1199
16	58.91	0.3566
17	62.84	0.1105
18	64.83	0.2986
19	65.99	0.0344
20	68.51	0.2790
21	70.39	0.0496
22	73.82	0.3552
23	77.79	0.1664
24	80.67	0.0199
25	83.39	0.2298
26	84.19	0.4996
27	86.01	0.6000
28	87.29	0.2608
29	95.74	0.3990
30	99.34	0.0060
31	101.52	0.4593
32	106.60	0.0689
33	107.04	0.0629
34	108.40	0.1383
35	111.75	0.2855
36	115.22	0.5465
37	118.67	0.2254
38	121.26	0.2905
39	123.41	0.1628
40	124.32	0.1791
41	129.24	0.0123
42	149.73	0.6337
43	174.95	2.1121
44	266.26	5.2191
45	285.81	111.0307

46	784.63	36.1231
47	1205.89	190.4693
48	1492.16	368.3204

**NO<sub>2</sub>/Ag<sub>16</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.50	0.3684
2	28.91	0.0641
3	32.00	0.5436
4	35.74	0.1156
5	38.57	0.1583
6	40.48	0.1505
7	42.11	0.3340
8	44.51	0.3821
9	48.89	0.5686
10	49.38	0.0844
11	51.44	0.0862
12	53.19	0.0691
13	54.16	0.0433
14	56.19	0.1814
15	56.72	0.1743
16	57.48	0.1204
17	59.55	0.4689
18	61.67	0.1895
19	62.36	0.6591
20	65.01	0.5591
21	67.97	0.6236
22	68.02	0.3415
23	69.87	0.9609
24	71.34	0.5779
25	73.56	0.1576
26	76.66	0.0476
27	79.08	0.1712
28	81.08	0.0475
29	81.50	0.3775
30	83.42	0.0978
31	87.01	0.7486
32	88.43	0.0473
33	90.60	0.0747
34	92.62	0.1676
35	96.58	0.1611
36	102.11	0.1639
37	106.64	0.0055



38	108.62	0.0297
39	117.79	1.0486
40	120.61	0.5482
41	121.40	0.0188
42	125.17	0.3279
43	139.34	0.0566
44	144.65	0.0832
45	147.99	0.2246
46	191.79	1.7146
47	205.56	15.8158
48	235.46	19.8767
49	773.87	4.8469
50	1120.80	343.4104
51	1347.05	132.3407

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**NO<sub>2</sub>/Ag<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.99	0.0140
2	19.16	0.0390
3	25.38	0.1988
4	28.54	0.1416
5	30.53	0.0566
6	32.93	0.2113
7	37.30	0.0691
8	37.69	0.2238
9	40.37	0.2602
10	44.24	1.2279
11	46.02	0.0842
12	46.51	0.6044
13	47.94	0.0795
14	51.66	0.9802
15	53.37	0.0901
16	56.09	0.2937
17	57.54	1.0908
18	59.15	0.1320
19	60.19	0.4284
20	61.55	0.2215
21	63.23	0.2176
22	64.63	0.6325
23	68.01	0.3024
24	70.50	0.5226
25	73.00	0.0974
26	74.39	0.4104

27	77.03	0.2380
28	77.89	0.1416
29	79.78	0.1493
30	81.40	0.2361
31	83.04	0.5627
32	85.40	0.4938
33	89.13	0.2703
34	93.70	0.0328
35	95.89	0.3408
36	98.07	0.1923
37	99.79	1.1133
38	104.85	0.6158
39	107.69	1.0208
40	108.49	0.0296
41	112.99	0.1490
42	116.37	0.1171
43	118.17	2.1835
44	119.81	0.1640
45	124.50	0.3544
46	127.62	3.3345
47	131.81	0.1777
48	134.54	1.5025
49	224.70	5.3902
50	246.44	27.5961
51	269.89	12.6114
52	782.44	4.3444
53	1181.58	233.1583
54	1328.24	63.6917

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**NO<sub>2</sub>/Ag<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.02	0.2155
2	16.88	0.8469
3	22.31	0.7682
4	24.95	0.0297
5	26.46	0.9181
6	32.71	0.9791
7	35.39	0.2220
8	39.54	0.0486
9	42.00	0.0914
10	42.87	0.0480
11	45.57	0.0873
12	46.42	0.0184

13	48.08	0.1468
14	50.29	0.1455
15	52.42	0.0378
16	54.41	0.1188
17	56.51	0.0610
18	57.31	0.2222
19	58.50	0.0469
20	61.26	0.2551
21	61.58	0.1291
22	64.61	0.5504
23	65.29	0.4630
24	66.00	0.5838
25	68.72	0.1939
26	70.13	0.6985
27	71.70	0.0713
28	72.80	0.9263
29	74.92	0.2719
30	77.88	0.4150
31	80.80	0.5639
32	81.90	0.6552
33	86.44	0.4071
34	87.28	0.1340
35	90.24	0.0168
36	93.33	0.0181
37	95.97	0.0224
38	97.29	0.0362
39	100.18	0.0374
40	103.74	0.2644
41	106.59	0.0146
42	107.94	0.0916
43	109.25	0.1093
44	112.45	0.1222
45	114.68	0.0449
46	116.88	0.4057
47	117.63	0.5847
48	120.17	0.5366
49	122.98	0.0683
50	128.65	0.0412
51	152.86	0.9831
52	179.51	1.4864
53	275.45	3.7073
54	288.50	81.8422
55	786.84	31.8445

56	1199.71	195.4102
57	1494.55	375.7744

<b>NO<sub>2</sub>/Ag<sub>19</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.69	0.1719
2	28.52	0.3878
3	29.64	0.4825
4	31.84	0.1937
5	35.13	0.2978
6	36.92	0.0400
7	37.55	0.2968
8	38.69	0.0319
9	40.32	0.0888
10	41.72	0.3214
11	42.92	0.4421
12	44.11	0.2011
13	46.04	0.1907
14	48.07	0.1945
15	51.71	0.4203
16	53.01	0.2509
17	54.24	0.6778
18	55.26	0.4483
19	56.40	0.5613
20	57.59	0.3266
21	57.91	0.1666
22	59.58	0.1680
23	61.79	0.1774
24	64.98	0.1269
25	65.65	0.2050
26	65.75	0.0539
27	68.24	0.1372
28	70.50	0.6277
29	71.81	0.1569
30	73.17	0.1960
31	75.81	0.1498
32	76.49	0.0265
33	80.15	0.6150
34	81.30	0.4020
35	82.37	0.1431
36	84.92	0.4248
37	87.46	0.3581
38	89.35	0.0628

39	93.62	0.2774
40	93.74	0.0238
41	95.29	0.2111
42	97.62	0.1303
43	100.18	0.0413
44	105.15	0.4287
45	106.22	1.0621
46	108.93	1.2652
47	110.37	0.2422
48	116.72	0.2115
49	121.39	0.6641
50	128.38	0.9872
51	130.09	0.3232
52	137.22	0.2863
53	145.04	0.4430
54	154.80	2.6264
55	160.69	6.7897
56	194.93	30.7588
57	249.03	39.4090
58	766.40	11.4265
59	1169.12	345.1911
60	1321.86	64.2206

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**NO<sub>2</sub>/Ag<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.03	2.3899
2	30.71	0.2201
3	32.70	0.0223
4	35.28	0.2191
5	36.29	0.0697
6	39.34	0.0682
7	39.52	0.2260
8	43.31	0.1209
9	43.78	0.1030
10	45.57	0.1400
11	46.31	0.1184
12	46.98	0.0266
13	49.36	0.0550
14	49.49	0.1786
15	51.11	0.0590
16	52.59	0.1987
17	53.47	0.1802
18	54.53	0.0563

19	55.50	0.0492
20	56.73	0.0793
21	57.64	0.0883
22	58.89	0.0420
23	60.53	0.0063
24	61.81	0.0332
25	63.72	0.2160
26	65.25	0.0599
27	68.42	0.0093
28	70.29	0.0566
29	72.29	0.0728
30	73.70	0.1186
31	74.59	0.4296
32	75.52	0.2532
33	77.14	0.1198
34	77.41	0.0455
35	78.53	0.0335
36	80.45	0.0349
37	80.81	0.1003
38	82.16	0.0167
39	84.76	0.0533
40	86.12	0.0254
41	89.36	0.1789
42	92.90	0.0345
43	94.77	0.1612
44	97.00	0.0664
45	100.72	0.0208
46	102.58	0.0564
47	105.87	0.0892
48	111.67	0.0856
49	118.40	0.0854
50	122.36	0.1925
51	128.36	0.3307
52	132.76	0.3135
53	133.35	0.3659
54	136.01	0.3848
55	140.75	0.2363
56	141.68	0.0806
57	153.28	0.7528
58	177.70	1.3779
59	272.07	20.2302
60	277.91	68.2076
61	790.59	27.1978

62	1214.77	266.6434
63	1488.41	460.8931

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**NO<sub>2</sub>/Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.09	0.1950
2	28.16	0.1017
3	32.38	0.1356
4	33.85	0.2543
5	36.52	0.2704
6	37.33	0.2844
7	38.51	0.1602
8	39.89	0.0743
9	40.97	0.3812
10	42.56	0.0635
11	43.47	0.0161
12	44.33	0.3282
13	44.46	0.0513
14	45.42	0.1173
15	48.62	0.1532
16	49.88	0.0142
17	51.27	0.4557
18	52.65	0.7999
19	53.74	0.0425
20	55.83	0.1565
21	56.49	0.3273
22	58.02	0.2221
23	58.83	0.1115
24	59.10	0.1383
25	60.78	0.0903
26	61.97	0.1333
27	63.42	0.2622
28	65.65	0.4884
29	66.43	0.3046
30	67.62	0.0563
31	69.62	0.1495
32	71.29	0.1066
33	72.34	0.1046
34	73.97	0.0293
35	76.06	0.1408
36	77.74	0.3404
37	81.44	0.0666
38	85.02	0.0166

39	86.36	0.7085
40	87.89	0.1986
41	90.39	0.3281
42	93.57	0.1798
43	94.43	0.1201
44	96.32	0.3961
45	97.62	0.0556
46	100.74	0.0518
47	102.22	0.7339
48	106.45	0.0241
49	107.56	0.2611
50	108.17	0.2600
51	109.49	0.4500
52	112.12	0.0891
53	114.79	1.1421
54	116.94	0.3030
55	118.36	0.0808
56	122.34	0.1298
57	124.34	0.4747
58	128.28	0.0215
59	129.10	0.0810
60	138.32	0.0032
61	161.15	3.3642
62	201.83	22.6075
63	239.40	31.9251
64	767.15	9.1522
65	1160.51	177.2821
66	1318.49	26.2817

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**NO<sub>2</sub>/Ag<sub>22</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.78	0.0596
2	25.71	0.2103
3	28.86	0.0424
4	34.39	0.0611
5	37.58	0.0452
6	39.20	0.0631
7	39.52	0.0135
8	41.86	0.1599
9	43.63	0.0386
10	43.77	0.0419
11	45.31	0.1164
12	46.03	0.1244



13	47.72	0.1625
14	48.59	0.2422
15	49.51	0.1210
16	50.09	0.0049
17	51.62	0.1121
18	52.51	0.5193
19	53.18	0.0186
20	53.58	0.1273
21	54.56	0.0859
22	55.81	0.0472
23	57.07	0.1521
24	59.18	0.2880
25	60.49	0.4525
26	61.75	0.1381
27	62.66	0.0395
28	63.52	0.3198
29	64.97	0.1096
30	66.68	0.4303
31	68.60	0.1291
32	70.56	0.1883
33	71.18	0.2587
34	72.99	0.0334
35	73.40	0.2510
36	75.08	0.0597
37	76.80	0.0476
38	77.66	0.1338
39	78.79	0.1746
40	79.72	0.4625
41	80.12	0.0571
42	81.74	0.0715
43	84.56	0.4618
44	85.16	0.2756
45	86.39	0.1372
46	86.98	0.0660
47	89.47	0.2043
48	91.86	0.1464
49	93.07	0.3551
50	98.13	0.1303
51	98.95	0.1535
52	102.45	0.0341
53	107.19	0.0679
54	116.35	0.3100
55	118.73	1.0704

56	123.03	0.1471
57	124.17	0.2248
58	128.96	0.7505
59	132.97	0.3459
60	137.32	0.0858
61	141.69	0.4997
62	143.43	0.1101
63	150.74	0.9482
64	191.98	2.6084
65	199.71	24.4354
66	256.98	19.2792
67	769.01	6.7556
68	1160.30	143.8688
69	1322.97	29.7444

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**SO<sub>2</sub>/Ag<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	178.76	41.0429
2	205.99	0.0603
3	256.48	13.3335
4	484.45	40.4649
5	815.95	173.3790
6	855.94	22.2171

---

**SO<sub>2</sub>/Ag<sub>2</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	42.88	7.8559
2	70.52	10.0398
3	103.04	2.3023
4	108.27	0.0692
5	235.81	32.8585
6	303.78	4.4904
7	414.92	9.9831
8	680.33	366.0497
9	924.87	174.3235

---

**SO<sub>2</sub>/Ag<sub>3</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	34.40	0.0329
2	53.28	6.8810
3	84.61	0.0001
4	95.99	0.3870
5	106.49	0.5815
6	119.44	21.4845
7	145.27	0.5603

8	267.19	21.2596
9	300.62	5.5693
10	424.62	112.0723
11	878.90	127.2179
12	897.40	83.2532

---

**SO<sub>2</sub>/Ag<sub>4</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	26.19	3.0409
2	63.08	0.0445
3	68.43	2.0861
4	70.28	6.5669
5	79.50	1.8916
6	89.81	3.3595
7	114.15	3.3519
8	126.39	1.7713
9	193.37	11.5676
10	216.66	8.3176
11	341.38	9.6497
12	342.21	62.1280
13	415.97	75.4887
14	677.83	43.0542
15	737.13	38.9998

---

**SO<sub>2</sub>/Ag<sub>5</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.48	0.4501
2	15.53	0.0027
3	31.55	2.9084
4	37.01	0.0394
5	44.15	0.5959
6	57.21	1.5142
7	64.52	0.1973
8	71.33	1.2705
9	98.20	0.3223
10	101.76	18.7081
11	112.98	2.5657
12	133.59	1.0703
13	143.24	0.2551
14	261.18	38.8392
15	292.67	8.2970
16	420.08	164.2706
17	871.83	86.9954
18	893.25	107.9067

<b>SO<sub>2</sub>/Ag<sub>6</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.35	0.0127
2	39.11	0.1093
3	46.17	1.3506
4	55.29	0.8517
5	64.27	0.9659
6	64.41	2.5825
7	66.16	6.0232
8	77.92	0.3138
9	88.28	0.0709
10	93.67	2.3130
11	101.05	1.3033
12	120.14	3.7682
13	123.23	0.5719
14	146.48	1.1184
15	186.71	17.2759
16	225.42	22.9507
17	363.64	2.3009
18	378.11	61.4182
19	401.71	61.6763
20	668.14	46.4562
21	726.43	36.7139

<b>SO<sub>2</sub>/Ag<sub>7</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.18	0.0073
2	32.08	0.1676
3	44.49	0.5471
4	48.50	0.7829
5	54.56	1.8048
6	62.74	0.5570
7	66.08	0.5745
8	70.28	0.0339
9	73.56	0.8635
10	76.78	0.3795
11	82.31	0.1957
12	84.03	0.0384
13	93.87	0.4245
14	98.34	0.4945
15	102.30	4.7105
16	123.92	0.7997
17	126.09	0.0703

18	127.39	0.7582
19	187.04	17.4834
20	235.69	16.4900
21	258.27	7.6712
22	413.38	54.2925
23	827.79	98.9359
24	897.04	35.0043

**SO<sub>2</sub>/Ag<sub>8</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.37	0.2871
2	33.97	0.0652
3	38.78	0.5900
4	45.28	1.0379
5	50.44	0.2912
6	51.38	0.3801
7	60.71	0.7148
8	64.40	2.0291
9	69.36	0.2835
10	74.01	0.1061
11	75.85	1.9062
12	84.14	1.8391
13	89.85	1.7892
14	94.32	0.1117
15	96.11	1.7991
16	102.15	2.1391
17	118.57	1.7210
18	129.53	1.3507
19	132.37	0.1912
20	193.45	6.8300
21	206.93	10.1902
22	243.42	6.4272
23	271.88	11.4436
24	317.05	70.0079
25	401.04	14.8890
26	690.98	37.4997
27	730.81	20.3174

**SO<sub>2</sub>/Ag<sub>9</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.27	0.0027
2	37.65	0.1470
3	44.43	0.5078
4	49.24	0.1823

5	50.03	0.1964
6	58.68	0.4548
7	58.80	0.8971
8	61.76	0.2315
9	65.67	0.3318
10	69.12	0.0332
11	74.55	0.0040
12	77.00	0.0068
13	78.08	0.1625
14	83.00	0.0527
15	83.11	1.0175
16	91.17	0.0860
17	92.59	0.2133
18	101.09	0.2896
19	102.75	1.0642
20	115.27	0.1735
21	120.51	0.2472
22	133.94	0.1243
23	140.88	0.3203
24	147.61	0.3969
25	162.76	4.0330
26	193.26	8.3126
27	194.57	13.8109
28	389.41	28.5933
29	806.60	25.8553
30	822.61	37.1736

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**SO<sub>2</sub>/Ag<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.39	0.1484
2	25.30	0.3039
3	28.41	2.0113
4	40.76	1.7218
5	42.33	1.7403
6	45.05	1.7193
7	49.34	0.1972
8	50.31	0.1380
9	55.79	0.3354
10	56.97	0.3194
11	61.92	0.5180
12	65.21	0.7963
13	68.95	0.3451
14	73.34	1.3642

15	76.43	0.1035
16	80.10	0.4924
17	85.88	0.2957
18	93.39	1.2564
19	95.14	0.1597
20	99.15	0.5501
21	104.27	0.3052
22	107.82	0.0120
23	113.76	0.8781
24	120.51	0.2579
25	124.92	0.7990
26	132.72	0.0326
27	258.80	5.4257
28	274.25	8.7756
29	286.19	45.6696
30	310.74	9.3435
31	384.17	72.7983
32	703.02	27.5257
33	752.44	32.9194

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**SO<sub>2</sub>/Ag<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.57	0.8869
2	25.22	0.0313
3	35.01	0.0458
4	36.62	0.0311
5	40.35	0.2356
6	42.33	0.4847
7	44.10	0.3425
8	49.20	0.1575
9	52.22	0.5464
10	54.14	0.7597
11	56.62	0.1348
12	57.69	0.5001
13	59.14	0.0808
14	61.85	0.2406
15	67.33	0.2698
16	70.77	0.0408
17	74.94	0.2799
18	75.05	0.2047
19	80.38	0.0609
20	87.30	0.3167
21	87.97	0.2317

22	92.20	0.1398
23	99.16	0.8468
24	104.64	3.5541
25	111.18	0.2461
26	114.24	0.0566
27	117.89	2.9588
28	122.27	0.7294
29	126.95	0.1633
30	142.20	0.8057
31	213.12	20.9528
32	241.63	25.1828
33	274.21	6.1907
34	411.47	62.8909
35	818.29	89.3342
36	895.35	20.5866

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**SO<sub>2</sub>/Ag<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.68	0.2060
2	22.63	0.7170
3	25.58	0.3948
4	32.44	0.2323
5	37.79	0.1231
6	38.82	0.1394
7	42.19	0.0684
8	46.28	0.4611
9	48.18	0.8280
10	51.21	0.5994
11	54.98	0.4901
12	57.50	0.1141
13	61.62	1.5267
14	64.20	0.3597
15	65.11	2.1679
16	67.71	1.2856
17	72.02	0.4970
18	75.31	1.1810
19	77.64	0.8133
20	78.72	1.0701
21	87.60	0.7793
22	91.73	0.3180
23	96.55	1.2556
24	98.38	0.6214
25	102.57	0.8198



26	108.04	0.4647
27	111.14	0.4213
28	115.63	0.4524
29	117.87	0.4677
30	123.26	2.0916
31	131.84	2.0191
32	140.18	1.8370
33	264.40	7.7364
34	273.43	7.6029
35	290.96	40.0170
36	349.88	28.6845
37	410.15	44.5149
38	711.23	51.8015
39	768.42	62.9440

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**SO<sub>2</sub>/Ag<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.02	0.0134
2	22.92	0.0799
3	27.73	0.2893
4	30.13	0.0583
5	32.32	0.1084
6	35.28	0.2383
7	39.41	0.0185
8	44.62	0.2323
9	45.77	0.1700
10	47.77	0.2968
11	51.23	0.0478
12	52.20	0.4698
13	54.35	0.0916
14	56.39	0.2915
15	61.43	0.8094
16	61.96	0.1700
17	63.76	0.1199
18	67.56	0.3136
19	73.55	0.1504
20	74.97	0.4523
21	77.73	0.1147
22	78.53	0.3646
23	79.06	0.3964
24	80.86	0.0852
25	88.25	0.1970
26	90.09	0.0693

27	97.63	1.1154
28	102.17	0.3533
29	105.42	0.9180
30	110.16	1.5527
31	112.92	0.8373
32	120.71	0.7489
33	125.39	2.3626
34	128.67	0.0777
35	130.49	0.2557
36	137.68	0.4025
37	154.32	17.6836
38	246.57	15.8566
39	263.05	4.8132
40	412.97	61.6408
41	820.44	59.2929
42	884.12	20.3741

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**SO<sub>2</sub>/Ag<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.36	0.0407
2	23.08	0.0761
3	29.35	0.0536
4	32.46	0.0683
5	36.11	0.1200
6	38.64	0.0908
7	43.11	0.1127
8	43.47	0.1901
9	47.68	0.2097
10	48.68	0.3647
11	51.15	0.1982
12	55.88	0.1254
13	57.13	0.6403
14	57.64	0.2111
15	61.56	0.1197
16	65.43	0.0462
17	67.27	0.2478
18	67.68	0.3477
19	72.92	1.0757
20	76.50	0.3686
21	77.88	0.4835
22	78.51	1.3317
23	82.43	0.3010
24	83.38	0.7506

25	87.92	0.5854
26	91.62	0.7017
27	95.14	0.2728
28	96.42	0.6189
29	98.66	0.2892
30	105.31	0.2836
31	106.20	0.2877
32	114.17	0.3523
33	116.82	0.8455
34	120.38	0.6211
35	132.05	0.5836
36	137.25	0.8794
37	140.63	0.3764
38	189.38	5.0102
39	209.99	6.9919
40	238.27	2.5056
41	307.19	10.9146
42	330.61	94.1243
43	407.75	7.1001
44	693.92	25.3321
45	736.44	14.1330

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**SO<sub>2</sub>/Ag<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.95	0.0474
2	27.44	0.0225
3	32.76	0.0374
4	36.32	0.0751
5	38.15	0.1128
6	39.29	0.1376
7	41.83	0.2408
8	43.63	0.0419
9	43.85	0.3631
10	48.93	0.0113
11	51.36	0.1572
12	52.68	0.2997
13	55.88	0.0978
14	57.23	0.1975
15	57.49	0.1380
16	61.03	0.2232
17	61.63	0.4390
18	64.04	0.2136
19	67.96	0.2707

20	69.47	0.4740
21	71.17	0.1131
22	74.30	0.4559
23	78.27	0.1077
24	79.51	0.0361
25	80.43	0.2082
26	81.63	0.4957
27	82.71	0.4013
28	84.82	0.1057
29	90.93	0.0888
30	97.91	0.0191
31	100.06	0.4681
32	104.32	0.2281
33	105.28	0.1338
34	109.34	1.8453
35	111.33	0.6508
36	117.63	1.4454
37	120.84	0.0114
38	123.27	0.1204
39	125.51	0.4163
40	128.37	0.4724
41	135.31	0.2363
42	167.07	3.5047
43	178.72	6.1295
44	206.22	12.3300
45	216.24	11.6015
46	394.74	33.1479
47	825.98	32.7888
48	831.33	7.9745

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**SO<sub>2</sub>/Ag<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.24	0.2400
2	24.01	0.1330
3	28.01	0.0113
4	31.39	0.1938
5	34.99	0.1217
6	36.92	0.1352
7	40.62	0.0872
8	41.58	0.0933
9	43.18	0.3848
10	44.68	0.7502
11	48.40	0.0436

12	50.03	0.5054
13	50.83	0.0878
14	52.31	0.0561
15	54.95	1.1318
16	58.01	1.2100
17	59.60	0.6570
18	61.78	1.1993
19	63.52	0.5811
20	66.11	3.9198
21	67.96	0.6411
22	68.46	0.0721
23	70.91	0.2166
24	72.39	0.4167
25	73.58	0.2004
26	77.87	0.1241
27	80.52	0.5063
28	82.90	0.1117
29	84.84	0.2198
30	88.18	0.3450
31	90.87	0.2386
32	96.18	0.0964
33	99.93	0.0550
34	101.93	0.1863
35	104.35	0.0481
36	108.57	0.3133
37	112.29	0.0751
38	115.05	0.5016
39	116.36	0.9748
40	119.48	0.0593
41	120.98	0.3553
42	126.73	0.4167
43	129.16	0.1134
44	135.18	0.2661
45	247.53	22.6746
46	259.07	12.1866
47	324.90	15.8966
48	343.48	25.2439
49	387.24	75.0380
50	690.82	22.3463
51	753.23	77.5202

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$\text{SO}_2/\text{Ag}_{17}$

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**Mode**

**Frequency**

**Infrared**

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1	18.14	0.2177
2	21.82	0.5859
3	24.77	0.0727
4	25.76	0.0358
5	30.40	0.0942
6	32.58	0.1531
7	36.94	0.0608
8	37.96	0.1308
9	39.62	0.2496
10	40.01	0.3330
11	43.08	0.1573
12	46.09	0.1493
13	46.84	0.2026
14	48.67	0.0831
15	50.86	0.0434
16	51.53	0.1061
17	56.98	0.2956
18	57.33	0.2520
19	58.78	0.1304
20	60.60	0.0349
21	64.71	0.2256
22	65.86	0.1831
23	66.95	0.5899
24	68.80	0.2446
25	70.85	0.1817
26	71.53	0.0998
27	74.59	0.7895
28	77.36	0.2894
29	77.91	0.0983
30	81.29	0.8990
31	83.18	0.4080
32	86.56	0.3890
33	90.69	0.5514
34	93.45	0.2362
35	95.53	0.1121
36	96.44	0.0754
37	99.74	0.0398
38	100.57	0.2303
39	106.16	0.0587
40	107.30	2.7817
41	111.57	0.4804
42	114.24	0.5166
43	117.99	0.3786

44	123.95	0.3203
45	125.43	0.1830
46	128.80	0.9095
47	140.55	3.0310
48	147.34	1.7262
49	149.61	6.6007
50	210.86	6.9980
51	252.90	7.7036
52	418.99	30.7035
53	785.27	62.5284
54	887.42	65.7969

**SO<sub>2</sub>/Ag<sub>18</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.49	0.2228
2	18.99	0.2592
3	26.10	0.0192
4	32.03	0.0065
5	34.32	0.1470
6	38.70	0.0279
7	39.54	0.0581
8	41.28	0.0382
9	45.41	0.4531
10	46.05	0.0023
11	49.74	0.0002
12	50.55	0.2680
13	51.94	0.1619
14	52.77	0.4332
15	53.76	0.4689
16	56.71	0.3263
17	57.88	0.0412
18	59.58	0.0004
19	60.56	0.2367
20	63.62	0.7154
21	64.16	0.7179
22	64.52	0.0284
23	67.94	0.2104
24	69.81	0.7769
25	70.78	0.0596
26	71.93	0.7092
27	74.36	0.1351
28	75.38	0.4999
29	77.70	0.1347

30	78.64	0.3796
31	86.66	0.5576
32	87.94	0.5593
33	92.97	0.5792
34	93.08	0.8176
35	93.96	0.2223
36	96.57	0.2045
37	97.99	0.1156
38	100.49	0.2041
39	101.25	0.3040
40	103.29	0.0929
41	105.53	0.3206
42	107.87	0.0004
43	110.04	0.3436
44	113.76	0.3243
45	121.25	1.1933
46	122.69	2.2626
47	124.01	0.1491
48	124.65	0.6554
49	133.04	0.2705
50	173.12	4.4164
51	173.53	4.4124
52	220.21	2.4104
53	312.19	4.1529
54	313.69	107.3190
55	417.94	7.1350
56	716.32	26.3127
57	764.35	19.7115

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**SO<sub>2</sub>/Ag<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	26.48	0.0116
2	30.90	0.0181
3	32.60	0.0322
4	35.40	0.0102
5	37.04	0.0515
6	39.02	0.1040
7	40.61	0.0616
8	43.42	0.0364
9	45.61	0.0378
10	45.92	0.0102
11	47.94	0.1373
12	48.81	0.0442



13	49.89	0.0089
14	50.75	0.1346
15	52.48	0.1530
16	53.06	0.1052
17	54.36	0.0439
18	54.72	0.0799
19	56.38	0.1780
20	58.67	0.2084
21	60.37	0.4251
22	62.70	0.1185
23	63.35	0.5465
24	64.27	0.1907
25	67.43	0.1264
26	68.64	0.1615
27	70.24	0.1322
28	72.20	0.0194
29	73.20	0.2225
30	75.37	0.1132
31	76.56	0.1295
32	77.87	0.1113
33	80.29	0.0709
34	81.12	0.4225
35	81.61	0.0523
36	83.75	0.4531
37	86.08	0.0597
38	89.35	0.4621
39	91.57	0.0527
40	95.15	0.1500
41	95.81	0.0721
42	98.70	0.2545
43	101.30	0.0094
44	104.84	0.1178
45	105.77	0.0589
46	107.27	0.0932
47	118.62	0.0573
48	120.81	0.6250
49	122.11	3.2487
50	132.43	0.7253
51	136.52	0.2892
52	137.16	0.3299
53	137.74	0.1204
54	145.97	0.1660
55	213.58	19.1081

56	226.27	3.4598
57	249.24	2.4585
58	407.98	32.2637
59	794.82	15.9851
60	867.46	73.2873

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**SO<sub>2</sub>/Ag<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.16	0.3153
2	23.59	0.0679
3	25.96	0.0412
4	31.20	0.0038
5	32.49	0.1122
6	34.01	0.0545
7	36.45	0.1006
8	38.94	0.0087
9	40.00	0.5815
10	42.78	0.0803
11	44.03	0.1531
12	45.74	0.0917
13	46.65	0.3027
14	47.71	0.5613
15	48.46	0.2259
16	50.44	0.1237
17	52.41	0.1233
18	53.86	0.2986
19	54.84	0.2266
20	56.13	0.1734
21	58.79	0.2341
22	61.39	0.4970
23	62.10	0.7679
24	62.56	0.4374
25	64.22	0.2799
26	64.39	0.3720
27	67.38	0.2191
28	68.67	0.2497
29	70.87	0.3976
30	72.33	0.2870
31	75.59	1.2178
32	77.36	0.2118
33	79.90	0.5896
34	81.26	0.2698
35	85.53	0.0085

36	86.58	0.0791
37	87.74	0.4819
38	90.77	0.2905
39	91.96	0.1817
40	96.35	0.1684
41	97.54	1.0066
42	101.06	0.2345
43	102.11	0.2595
44	104.52	0.4972
45	108.33	0.5071
46	109.64	0.1675
47	111.43	0.0544
48	114.22	0.1524
49	115.69	0.1223
50	118.84	0.4259
51	121.63	0.7028
52	125.95	0.4320
53	129.73	0.4204
54	134.63	0.1153
55	140.88	0.3072
56	175.08	5.4250
57	183.40	4.1947
58	213.48	0.3881
59	291.52	44.6923
60	302.75	66.6845
61	427.49	6.0332
62	697.31	22.5567
63	748.22	12.4514

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**SO<sub>2</sub>/Ag<sub>21</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	25.20	0.1993
2	30.97	0.0700
3	32.97	0.0063
4	33.94	0.2785
5	36.49	0.1891
6	37.16	0.0405
7	39.23	0.2204
8	40.02	0.0323
9	41.29	0.0061
10	41.68	0.0270
11	42.91	0.0849
12	46.12	0.0573

13	46.67	0.0646
14	47.93	0.0540
15	48.63	0.2144
16	50.11	0.1434
17	51.58	0.0793
18	53.22	0.0041
19	53.71	0.3258
20	54.10	0.1325
21	54.99	0.3488
22	57.99	0.5590
23	59.76	0.0399
24	60.35	0.0794
25	61.62	0.3469
26	63.36	0.0922
27	64.45	0.2743
28	65.80	0.1677
29	68.15	0.1501
30	69.08	0.0915
31	69.97	0.0172
32	70.52	0.1829
33	72.19	0.0216
34	75.63	0.0034
35	76.50	0.2428
36	77.89	0.0583
37	80.38	0.0230
38	82.96	0.0135
39	87.51	0.0896
40	89.10	0.0931
41	92.10	0.2967
42	93.59	0.0854
43	94.52	0.3304
44	96.63	0.2870
45	97.66	0.1160
46	100.33	0.3175
47	102.38	0.0422
48	104.19	0.8681
49	104.81	0.0727
50	107.04	0.2111
51	109.66	0.2899
52	112.31	0.1278
53	114.76	0.4014
54	117.26	0.0129
55	119.53	0.5147

56	125.54	0.7218
57	126.74	0.5287
58	127.02	0.3957
59	129.71	0.0015
60	135.65	0.0345
61	163.47	1.3889
62	204.07	16.0160
63	216.16	15.1055
64	401.03	64.2676
65	773.90	63.1468
66	890.52	10.3511

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**SO<sub>2</sub>/Ag<sub>22</sub>**

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Mode	Frequency	Infrared
1	16.22	0.3002
2	21.98	0.0461
3	25.62	0.3006
4	28.77	0.2589
5	29.61	0.6520
6	33.91	0.4826
7	35.78	0.0957
8	37.00	0.6963
9	38.55	0.0451
10	42.35	0.9399
11	43.62	0.2203
12	44.47	0.3735
13	45.31	0.1354
14	47.04	0.1087
15	48.66	0.2384
16	49.13	0.1458
17	49.80	0.0699
18	50.27	0.7439
19	52.50	0.4189
20	53.02	0.5730
21	54.75	0.4531
22	56.43	0.3338
23	58.56	0.0997
24	59.43	0.2554
25	60.22	0.0732
26	61.90	0.0581
27	63.35	0.1041
28	64.50	0.4846
29	65.20	0.3548

30	67.10	0.5236
31	68.67	0.2788
32	70.03	0.2061
33	70.36	0.1592
34	71.94	0.0237
35	75.38	0.1050
36	76.02	0.0595
37	76.98	0.3018
38	78.26	0.0869
39	79.58	0.0829
40	80.26	0.1184
41	81.49	0.2153
42	84.40	0.0320
43	85.86	0.1378
44	87.93	0.3152
45	89.26	0.3592
46	91.38	0.0727
47	93.04	0.2264
48	96.20	0.2132
49	98.36	0.2077
50	101.97	0.0552
51	102.98	0.1102
52	106.40	0.0889
53	109.14	0.2946
54	114.25	0.6295
55	116.49	0.2151
56	120.90	0.6192
57	123.55	0.1002
58	128.71	0.5444
59	130.70	0.0727
60	139.58	0.0931
61	146.76	0.1234
62	148.86	0.1393
63	180.33	10.3998
64	228.23	4.5678
65	329.19	45.4512
66	353.91	77.5566
67	420.04	8.4861
68	673.15	28.4554
69	731.17	36.5529

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<b>H<sub>2</sub>O</b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	1571.22	112.0832

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2	3763.76	0.0008
3	3952.93	36.9162

<b>H<sub>2</sub>O_Ag<sub>1</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	112.23	310.9055
2	192.41	5.2124
3	293.31	17.4905
4	1575.72	116.5682
5	3728.67	60.1537
6	3911.57	84.2807

<b>H<sub>2</sub>O_Ag<sub>2</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	46.25	6.1075
2	46.27	12.4957
3	147.20	0.2191
4	214.44	344.7970
5	262.38	16.9897
6	408.06	36.6613
7	1596.98	152.3239
8	3764.56	1.2573
9	3930.16	116.6984

<b>H<sub>2</sub>O_Ag<sub>3</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.72	2.9330
2	44.53	9.3718
3	47.69	0.0137
4	58.26	0.7324
5	98.10	2.0259
6	136.17	1.2307
7	262.21	358.3425
8	280.32	12.7710
9	427.35	50.1007
10	1603.07	186.6189
11	3777.68	11.9791
12	3937.14	112.6151

<b>H<sub>2</sub>O_Ag<sub>4</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	23.22	2.1805
2	28.93	1.1115
3	43.60	8.6771
4	67.37	2.9915
5	72.96	0.2036
6	86.65	0.0902
7	113.25	0.0073
8	127.22	9.6270

9	143.47	0.0565
10	256.30	337.7309
11	291.08	8.3552
12	436.87	26.2245
13	1599.21	203.9246
14	3784.61	19.5822
15	3944.39	91.2306

<b>H<sub>2</sub>O_Ag<sub>5</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.82	1.3328
2	20.17	0.0522
3	23.21	0.0000
4	37.89	4.3464
5	57.56	2.0593
6	63.30	0.4784
7	63.48	0.4682
8	91.01	0.0629
9	114.31	0.3320
10	126.67	0.3347
11	127.91	5.2737
12	145.30	3.7848
13	196.04	256.3349
14	253.13	0.2112
15	371.37	4.1033
16	1574.95	295.4680
17	3722.74	40.7622
18	3899.20	24.5255

<b>H<sub>2</sub>O_Ag<sub>6</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.77	2.4771
2	23.97	0.0071
3	27.39	0.3620
4	34.71	0.3248
5	39.77	4.5753
6	50.93	0.2896
7	61.38	0.2507
8	67.20	0.4648
9	72.93	0.8357
10	98.93	0.0612
11	104.16	0.0293
12	107.84	0.0144
13	110.78	0.6544
14	143.44	7.7558
15	157.04	8.4632
16	185.20	274.6418
17	238.77	2.2770



18	363.04	18.9161
19	1580.67	298.1839
20	3743.28	19.4154
21	3915.09	44.2827

<b>H<sub>2</sub>O_Ag<sub>7</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.53	9.6566
2	24.75	0.4275
3	28.62	4.7461
4	37.86	0.0005
5	39.67	0.5232
6	61.52	0.2929
7	63.34	0.4687
8	69.05	0.0000
9	74.77	0.0361
10	75.20	0.1830
11	75.45	0.0433
12	81.40	0.0087
13	88.59	0.0000
14	89.55	0.0014
15	95.02	0.1742
16	118.27	0.0128
17	121.71	0.1769
18	124.55	0.0075
19	219.05	278.7002
20	252.99	17.1140
21	396.53	14.6387
22	1596.80	204.3208
23	3762.90	0.3350
24	3927.46	85.4220

<b>H<sub>2</sub>O_Ag<sub>8</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	27.17	4.6899
2	27.40	10.6777
3	36.38	0.5601
4	40.12	0.1121
5	46.60	1.3798
6	48.82	0.3661
7	55.09	0.0143
8	56.98	0.1048
9	59.99	0.0461
10	60.31	0.3410
11	63.10	0.1993
12	69.10	0.5061
13	73.57	0.0480
14	88.40	0.2541

15	88.65	0.0076
16	90.20	0.0044
17	100.60	0.9445
18	114.37	0.1031
19	120.53	0.0429
20	121.60	0.1168
21	129.16	2.4017
22	159.08	210.4818
23	240.26	9.8957
24	369.07	16.9959
25	1587.55	185.7841
26	3757.35	0.7511
27	3925.38	80.8133

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<b>H<sub>2</sub>O_Ag<sub>9</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.33	5.6398
2	25.63	1.1419
3	33.01	0.0499
4	38.49	0.0877
5	39.62	0.5775
6	41.59	0.0144
7	48.63	0.2112
8	51.56	0.0897
9	54.49	0.8126
10	55.83	0.1575
11	57.56	0.0012
12	65.26	0.1783
13	69.15	0.1381
14	70.69	0.0377
15	84.10	0.0247
16	85.66	0.1729
17	86.98	0.0091
18	92.05	0.1738
19	104.20	0.0208
20	111.64	0.1044
21	114.15	1.8605
22	117.75	1.4404
23	120.31	0.1410
24	129.52	0.6264
25	212.23	206.1236
26	239.00	46.8811
27	356.85	4.7326
28	1583.22	283.2364
29	3734.51	20.1257
30	3906.51	37.5407

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**H<sub>2</sub>O\_Ag<sub>10</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.71	0.0343
2	26.48	0.2440
3	29.04	0.5765
4	31.88	0.1481
5	36.87	0.0571
6	41.11	0.0161
7	49.87	0.0713
8	54.11	0.2882
9	56.21	0.4800
10	57.54	0.7218
11	58.42	0.5501
12	64.53	0.6702
13	66.32	0.2589
14	72.77	3.6454
15	75.49	0.4608
16	80.27	0.0658
17	82.15	1.3443
18	86.56	0.2222
19	88.14	0.1673
20	98.59	0.1759
21	100.01	0.1900
22	109.30	0.5434
23	123.17	1.0377
24	124.44	4.1321
25	126.41	1.9507
26	133.66	22.2675
27	147.08	13.3677
28	225.39	15.9768
29	415.57	226.0564
30	496.44	171.9783
31	1590.92	27.7919
32	3644.15	61.2477
33	3805.11	11.3551

<b>H<sub>2</sub>O_Ag<sub>11</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.18	7.6001
2	18.90	0.9123
3	23.56	2.7948
4	31.00	0.0684
5	34.54	0.2835
6	39.85	0.1155
7	42.19	0.1471
8	44.78	0.2921
9	49.01	0.1418
10	55.71	0.0129

11	56.86	0.3070
12	59.38	0.2540
13	61.64	0.9184
14	64.83	0.2951
15	69.69	0.1312
16	73.98	0.1810
17	74.17	0.2360
18	77.08	0.1619
19	80.63	1.8530
20	85.93	1.8890
21	86.64	36.0414
22	93.94	0.1161
23	98.18	0.0430
24	100.15	0.3792
25	107.51	0.0367
26	108.88	1.2223
27	110.84	0.0217
28	116.45	0.1615
29	120.06	3.7001
30	129.74	0.0449
31	205.37	205.6331
32	250.00	10.0015
33	383.45	30.2058
34	1584.07	267.9199
35	3743.57	8.6024
36	3912.99	53.5041

<b>H<sub>2</sub>O_Ag<sub>12</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	25.13	0.6243
2	28.29	1.5475
3	32.02	0.6524
4	37.00	0.6871
5	38.00	0.6884
6	39.56	0.3600
7	40.51	0.1227
8	46.40	0.3024
9	47.71	0.8410
10	51.33	0.1991
11	54.13	0.1921
12	55.60	0.1167
13	56.87	0.4750
14	59.06	0.4902
15	61.47	0.1332
16	69.44	0.7149
17	71.04	0.1023
18	73.55	0.0899

19	76.65	0.2589
20	77.81	0.2355
21	78.04	0.3437
22	80.71	0.1043
23	88.20	2.4019
24	92.96	0.4857
25	101.12	0.2962
26	102.10	3.5928
27	108.89	0.5199
28	110.73	20.2411
29	117.74	0.9715
30	117.85	52.3971
31	121.12	2.8128
32	125.92	1.5889
33	129.95	0.0533
34	140.94	24.8578
35	230.82	3.1210
36	358.84	43.9324
37	1572.35	292.5059
38	3707.71	41.6497
39	3886.75	63.9824

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<b>H<sub>2</sub>O_Ag<sub>13</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.58	6.9726
2	27.29	1.2159
3	33.00	0.1660
4	35.20	0.2373
5	38.64	1.9513
6	40.58	0.1525
7	45.50	0.4062
8	47.70	0.8377
9	48.88	1.4957
10	50.68	0.8246
11	52.24	0.1976
12	54.42	0.2008
13	55.08	0.0313
14	57.85	0.1304
15	59.65	0.0600
16	62.48	0.0249
17	63.63	0.0327
18	66.16	0.0269
19	68.53	0.1806
20	74.57	0.0658
21	76.09	0.0418
22	79.50	0.0569
23	80.08	0.0135

24	84.72	0.0340
25	86.48	0.0644
26	92.94	0.0719
27	100.13	0.0183
28	100.68	0.0350
29	106.26	0.1224
30	109.64	0.3356
31	114.26	0.5118
32	122.40	0.2839
33	125.53	0.3441
34	128.97	0.5757
35	132.91	0.4261
36	167.01	85.4308
37	220.49	12.1397
38	307.97	90.9967
39	414.14	144.5540
40	1568.98	157.7962
41	3646.91	158.9637
42	3846.18	138.0336

<b>H<sub>2</sub>O_Ag<sub>14</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.37	6.8332
2	22.76	2.9957
3	30.38	0.2647
4	31.87	1.4773
5	35.81	0.2601
6	39.05	0.0734
7	40.65	0.5094
8	42.20	0.6747
9	44.40	0.0150
10	48.59	0.3380
11	48.94	0.4910
12	51.43	0.6728
13	55.52	0.3787
14	56.36	0.0074
15	59.16	0.7953
16	61.39	0.3708
17	63.48	0.0346
18	65.20	0.2748
19	66.47	0.0542
20	68.21	0.2215
21	71.07	1.7791
22	72.33	10.4910
23	72.68	1.9844
24	75.20	3.8561
25	75.69	15.7937

26	84.91	0.5018
27	91.11	0.2764
28	94.58	0.4161
29	96.18	0.3077
30	98.44	0.2475
31	99.40	0.0953
32	102.33	0.2197
33	104.82	0.0322
34	113.83	0.7066
35	117.65	0.1602
36	119.63	0.5742
37	122.98	0.4180
38	136.84	0.2623
39	141.53	0.4188
40	184.74	110.9816
41	242.66	2.6206
42	380.98	18.7171
43	1586.73	255.4760
44	3745.74	2.1534
45	3913.56	53.5044

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<b>H<sub>2</sub>O_Ag<sub>15</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.33	12.4206
2	19.48	3.6319
3	23.25	0.1760
4	24.83	0.0748
5	31.63	0.0642
6	35.43	0.0515
7	37.36	0.8467
8	42.92	0.3507
9	45.65	0.1978
10	46.39	0.5395
11	50.88	0.4330
12	51.31	1.3279
13	53.21	0.1517
14	54.65	0.4250
15	54.92	5.7994
16	57.24	0.0798
17	58.65	1.2221
18	62.27	0.3883
19	64.16	0.1566
20	65.35	0.0478
21	68.03	0.0763
22	71.00	0.4142
23	71.08	0.1903
24	73.00	0.0000

25	75.23	0.3647
26	76.08	0.0333
27	77.05	0.0487
28	84.21	0.0150
29	85.21	0.1516
30	88.54	0.7491
31	94.79	0.1000
32	94.82	0.2071
33	101.21	0.0175
34	101.82	0.0005
35	107.62	0.1156
36	108.53	0.0039
37	109.98	0.2121
38	114.84	0.5007
39	120.75	0.9951
40	122.39	0.0933
41	124.34	0.0797
42	135.85	0.1125
43	199.61	165.7382
44	244.57	10.2932
45	375.04	27.7445
46	1588.80	271.1133
47	3752.43	2.5352
48	3920.25	62.4119

<b>Mode</b>	<b>H<sub>2</sub>O_Ag<sub>16</sub></b>	
	<b>Frequency</b>	<b>Infrared</b>
1	17.92	0.2259
2	24.91	0.2011
3	27.62	0.0309
4	32.71	0.1474
5	35.58	0.6631
6	39.55	0.1122
7	42.18	0.3493
8	43.25	0.3316
9	44.47	0.2027
10	45.93	2.5419
11	47.66	0.1947
12	48.91	0.3929
13	51.42	0.0848
14	52.10	0.1245
15	52.74	0.4417
16	56.11	0.2090
17	57.24	0.0971
18	58.19	0.3865
19	60.86	0.0515
20	62.31	0.0325



21	64.73	0.0865
22	65.37	0.0453
23	69.95	0.0390
24	70.31	0.0078
25	71.77	0.0586
26	73.09	0.0388
27	74.85	0.4764
28	83.29	0.2073
29	84.55	0.0880
30	86.48	0.1137
31	90.55	0.0704
32	92.50	0.0980
33	96.90	0.1811
34	100.55	0.0497
35	104.48	0.1234
36	107.40	0.3001
37	109.84	0.0915
38	110.38	0.2087
39	114.33	0.3533
40	117.82	0.3768
41	121.09	0.4195
42	122.09	0.0392
43	128.31	0.7942
44	135.27	0.0542
45	203.00	4.0657
46	259.80	29.4748
47	321.81	177.6405
48	364.28	14.9907
49	1581.63	208.8382
50	3698.65	3.0739
51	3869.88	73.9814

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<b>H<sub>2</sub>O_Ag<sub>17</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.75	0.0317
2	20.66	0.0975
3	22.60	0.0763
4	28.37	3.9684
5	31.46	2.2858
6	35.23	2.6472
7	35.90	1.2395
8	36.41	0.1970
9	43.88	0.2302
10	44.47	0.2330
11	45.19	0.2488
12	46.60	0.3795
13	48.11	0.1052

14	49.47	1.5980
15	51.76	0.0320
16	56.19	0.0015
17	56.57	0.4408
18	59.56	0.0115
19	61.31	0.0358
20	63.84	0.9075
21	64.96	0.4375
22	67.01	0.5624
23	67.68	0.1695
24	70.31	0.5698
25	70.90	0.3982
26	73.27	0.0413
27	73.45	0.1142
28	75.56	0.0223
29	75.78	0.2811
30	78.51	0.4261
31	79.22	0.1458
32	80.56	0.0400
33	91.98	0.8564
34	93.32	0.0342
35	94.69	0.0182
36	96.32	0.0170
37	99.87	0.0039
38	103.46	0.1073
39	107.59	0.0080
40	109.44	0.0001
41	113.26	0.1398
42	114.57	0.1212
43	120.27	0.0184
44	120.64	0.1165
45	123.08	0.7314
46	123.21	0.3367
47	129.23	1.3620
48	133.20	0.0766
49	224.95	202.3791
50	263.68	10.7450
51	399.64	8.0778
52	1595.98	278.6279
53	3767.56	5.9887
54	3929.35	73.3169

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<b>H<sub>2</sub>O_Ag<sub>18</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.49	0.1827
2	23.83	0.8834
3	25.11	0.8539

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4	29.96	0.7418
5	30.09	0.6773
6	32.62	2.3936
7	34.52	0.2478
8	35.53	3.7160
9	38.41	0.0004
10	41.87	0.2053
11	42.61	0.1290
12	48.29	0.3560
13	48.39	0.0169
14	51.84	0.0120
15	52.28	0.0731
16	54.31	0.1364
17	54.69	0.0416
18	57.90	0.5041
19	60.56	0.0402
20	62.13	0.4835
21	62.17	0.0157
22	63.11	0.2682
23	65.41	0.1588
24	67.16	0.3786
25	70.79	0.5764
26	73.20	0.2335
27	73.25	0.2770
28	75.88	0.0000
29	76.51	0.3801
30	79.96	0.4322
31	80.39	0.6852
32	86.28	0.2159
33	87.02	0.2112
34	91.65	0.2890
35	92.11	0.0894
36	94.28	0.0204
37	94.72	0.0080
38	105.73	0.1260
39	106.89	0.2205
40	108.40	0.3772
41	109.10	0.1310
42	110.58	0.1346
43	111.32	0.5328
44	112.26	0.8144
45	114.60	0.9162
46	114.97	0.3628
47	116.35	0.0391
48	119.28	0.2387
49	121.86	0.4101

50	123.53	0.1057
51	127.39	0.0596
52	218.66	186.6297
53	254.25	9.1984
54	390.36	9.5759
55	1593.41	251.8619
56	3761.96	5.4102
57	3925.45	73.1878

<b>H<sub>2</sub>O_Ag<sub>19</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.30	2.5584
2	32.93	0.0152
3	35.05	0.8670
4	36.42	1.9309
5	38.33	0.0178
6	38.78	0.2731
7	38.96	0.0266
8	39.88	1.1107
9	40.70	0.0722
10	42.53	0.8054
11	44.62	0.1096
12	44.96	0.0021
13	46.60	0.0071
14	48.06	0.2726
15	48.82	0.0030
16	52.19	0.0001
17	52.20	0.0107
18	55.60	0.0370
19	56.77	0.0709
20	57.77	0.2316
21	59.00	0.4755
22	59.71	0.1816
23	60.69	0.6537
24	64.78	0.0982
25	65.26	0.1378
26	65.46	0.1230
27	66.69	0.0030
28	70.37	0.3698
29	71.03	0.2561
30	72.72	0.7328
31	73.74	1.2935
32	74.06	1.5425
33	76.80	0.2840
34	78.63	0.0082
35	79.63	0.1721
36	80.44	0.0106

37	80.57	0.0655
38	84.27	0.0073
39	92.41	0.1854
40	92.94	0.0860
41	93.43	0.0297
42	95.70	1.2019
43	99.08	0.0011
44	99.98	1.2237
45	105.10	0.1439
46	105.95	0.0050
47	112.17	0.0019
48	117.82	2.8315
49	121.23	0.1531
50	131.33	17.6540
51	132.60	1.0208
52	137.60	0.7820
53	138.82	0.1118
54	142.71	81.8433
55	144.09	29.2280
56	239.64	1.4434
57	362.07	3.7982
58	1586.29	245.6635
59	3754.88	0.9902
60	3921.99	54.4735

	<b>H<sub>2</sub>O_Ag<sub>20</sub></b>	
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	19.14	0.3474
2	21.52	4.4792
3	28.89	4.8903
4	29.35	0.0762
5	32.02	0.0680
6	39.27	0.0752
7	41.20	0.0470
8	41.92	0.1998
9	43.78	0.0434
10	44.03	0.0645
11	45.40	0.0511
12	48.97	0.0286
13	49.90	0.0731
14	51.29	0.0672
15	53.13	0.1229
16	54.26	0.5798
17	55.53	0.2380
18	56.14	0.0588
19	58.11	0.1679
20	58.82	0.0971

21	61.32	0.0349
22	61.59	0.0983
23	63.13	0.1503
24	63.79	0.0019
25	64.50	0.3913
26	66.33	0.1717
27	68.44	0.0508
28	70.30	0.1204
29	71.61	0.0113
30	71.94	0.0849
31	72.63	0.1748
32	74.41	0.2565
33	77.76	0.4509
34	78.00	0.4204
35	79.17	0.0888
36	83.63	7.3791
37	85.83	2.4631
38	87.63	0.1381
39	90.11	0.0481
40	91.16	0.6990
41	92.22	0.0564
42	94.01	0.0729
43	95.61	0.0156
44	104.78	0.8747
45	106.58	0.1517
46	107.25	0.0582
47	108.40	0.2518
48	110.41	0.3424
49	111.61	0.1385
50	112.14	0.5017
51	115.79	0.0262
52	117.33	0.4334
53	121.95	0.0125
54	127.61	0.0509
55	128.13	1.0576
56	129.68	0.5790
57	129.77	0.0628
58	177.95	281.0772
59	236.42	1.2611
60	370.51	2.5507
61	1590.67	230.2434
62	3749.19	0.9732
63	3914.91	42.7718

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	$\text{H}_2\text{O\_Ag}_{21}$	
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.56	2.8055

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2	28.64	0.8884
3	29.34	0.1113
4	31.28	0.4708
5	34.94	0.6628
6	35.93	0.7104
7	37.58	1.5794
8	39.36	0.0464
9	40.15	0.0117
10	42.21	0.0515
11	44.47	0.1426
12	45.80	0.0188
13	46.09	0.0054
14	46.72	0.1754
15	47.79	0.0208
16	49.94	0.1662
17	50.96	0.6662
18	51.22	0.5501
19	52.46	0.1217
20	53.63	0.0095
21	54.71	0.1650
22	55.73	0.2757
23	56.16	0.1510
24	56.50	0.0808
25	57.34	0.3132
26	59.03	0.0299
27	60.23	0.0896
28	61.90	0.1113
29	64.72	0.1530
30	67.75	0.1164
31	68.47	0.1670
32	70.19	0.0853
33	70.85	0.0937
34	71.75	0.0626
35	72.68	0.0626
36	76.19	0.0679
37	78.19	0.0027
38	83.48	0.1565
39	86.52	0.0184
40	87.40	0.0128
41	89.96	0.0803
42	91.88	0.0809
43	92.25	0.1274
44	94.07	0.0197
45	95.51	0.0632
46	98.73	0.0247
47	102.23	0.0463

48	103.38	0.2634
49	105.35	0.2410
50	105.86	0.4569
51	107.81	1.5895
52	110.19	0.5398
53	116.14	0.7478
54	121.74	0.1419
55	122.98	2.3785
56	124.16	2.3923
57	125.16	21.5474
58	126.27	6.4797
59	129.47	3.9501
60	130.39	1.1794
61	211.48	50.3643
62	359.14	604.5357
63	412.34	92.4939
64	1581.43	77.5417
65	3667.42	122.8957
66	3836.93	11.8700

<b>H<sub>2</sub>O_Ag<sub>22</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.35	0.1081
2	28.24	0.0194
3	29.54	0.1489
4	31.18	0.1150
5	33.93	0.2101
6	35.30	0.2080
7	37.82	0.0408
8	39.88	0.1780
9	40.30	0.2600
10	40.63	0.2310
11	44.12	0.1217
12	44.83	0.0450
13	46.28	0.1010
14	46.77	0.4087
15	47.78	0.2743
16	48.04	0.1094
17	48.95	0.1108
18	50.19	0.1144
19	52.04	0.3146
20	52.57	0.1646
21	54.67	0.0151
22	55.66	0.0657
23	56.31	0.1263
24	57.97	0.0592
25	59.15	0.0226



26	61.60	0.0747
27	61.92	0.1084
28	63.08	0.0120
29	65.06	0.2104
30	66.22	0.0820
31	66.86	0.0973
32	68.57	0.1404
33	70.72	0.1770
34	71.83	0.0505
35	72.16	0.0211
36	72.72	0.1711
37	75.75	0.0159
38	77.02	0.1985
39	78.21	0.0278
40	80.17	0.2309
41	82.10	0.0592
42	84.14	0.0522
43	84.71	0.0179
44	85.18	0.4904
45	87.84	0.0490
46	89.87	0.0126
47	90.97	0.0531
48	93.32	0.0271
49	98.69	0.2871
50	100.17	0.1433
51	103.21	0.1760
52	105.88	0.1900
53	108.82	0.3578
54	118.09	1.6524
55	119.04	0.3071
56	123.48	0.1551
57	127.59	0.8181
58	129.93	0.2949
59	130.49	0.3012
60	137.99	16.2754
61	140.78	34.0366
62	142.41	18.8461
63	160.08	0.5109
64	212.06	38.2014
65	364.49	478.1125
66	440.72	118.0977
67	1601.53	18.3642
68	3666.59	56.1038
69	3828.57	24.2520

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**Table S4**

Vibrational Frequency which are computed by M06-2X/SDD method for CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, and SO<sub>2</sub> gases; isolated silver clusters Au<sub>n</sub> (n=1-20), and gas/cluster structures at M06-2X/SDD level of theory

<b>Au<sub>2</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	153.9	0.0000

  

<b>Au<sub>3</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.03	0.1522
2	6.03	0.1522
3	89.3	0.0000
4	125.23	7.1513

  

<b>Au<sub>4</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	30	0.0532
2	53.92	0.0000
3	62.06	2.7702
4	82.49	0.0000
5	127.01	9.9663
6	142.08	0.0000

  

<b>Au<sub>5</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.05	0.0000
2	29.42	0.0602
3	48.94	0.1679
4	57.47	0.1825

5	77.69	0.2736
6	86.39	0.1083
7	106.82	0.0169
8	119.28	0.5828
9	147.21	4.7839

**Au<sub>6</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	28.98	0.0004
2	29.19	0.0000
3	32.31	0.1507
4	54.64	0.1871
5	55.63	0.1951
6	71.72	0.6645
7	72.24	0.6376
8	95.51	0.0000
9	103.81	0.0000
10	113.64	0.0001
11	155.59	9.7526
12	155.9	9.7491

**Au<sub>7</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.24	0.0046
2	18.94	0.1191
3	26.23	0.0048
4	30.89	0.1279
5	32.74	0.0077
6	45.16	0.0268
7	53.99	0.3335
8	67.62	0.3774
9	72.82	0.1651
10	89.83	0.1339
11	95.36	0.1068
12	97.14	0.0766
13	126.52	1.4405
14	143.57	7.2485
15	158.91	6.4003

**Au<sub>8</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.12	0.0000
2	23.35	0.0000
3	30.84	0.3323
4	33.99	0.0000
5	34	0.0000
6	36.94	0.0000

7	46.78	0.0000
8	55.08	0.3049
9	55.12	0.3047
10	74.14	0.0000
11	78.03	0.0000
12	90.69	1.1856
13	90.7	1.1871
14	108.61	0.0000
15	117.92	0.0000
16	154.11	15.5456
17	154.12	15.5420
18	170.78	0.0000

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**Au<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.17	0.0000
2	13.39	0.0203
3	27.93	0.0770
4	29.8	0.0426
5	31.69	0.0647
6	33.29	0.0000
7	36.09	0.0085
8	42.36	0.0036
9	45.47	0.0153
10	47.81	0.0065
11	63.83	0.0003
12	66.87	0.0313
13	69.22	0.1106
14	82.19	1.1871
15	82.69	0.0968
16	91.78	0.0446
17	107.37	0.0000
18	118.52	0.1561
19	143.71	9.4116
20	144.59	7.3685
21	159.37	1.3295

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**Au<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.11	0.0000
2	14	0.0176
3	21.9	0.0000
4	25.84	0.0232
5	29.11	0.0000
6	32.46	0.0881
7	39.57	0.0000

8	43.56	0.0000
9	44.6	0.1013
10	48.91	0.0000
11	58.02	0.0705
12	66.7	0.3054
13	67.4	1.2874
14	68.45	0.0000
15	72.78	0.0000
16	77.4	0.0000
17	87.01	0.0000
18	87.78	0.0044
19	98.82	0.0000
20	105.23	0.5995
21	115.72	3.1312
22	132.57	0.0000
23	133.14	3.6944
24	134.27	0.0000

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**Au<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.53	0.0002
2	12.57	0.0004
3	15.56	0.0282
4	21.79	0.0447
5	27.82	0.0379
6	29.37	0.0035
7	33.86	0.0004
8	36.15	0.0094
9	42.34	0.0596
10	43.87	0.0110
11	46.46	0.0572
12	49	0.0849
13	54.22	0.3032
14	59.99	0.0606
15	63.02	0.0958
16	71.56	0.0745
17	74.34	0.3893
18	79.79	0.6336
19	83.54	0.0632
20	87.75	0.2042
21	99.83	0.1785
22	105.95	0.0504
23	111.35	3.6214
24	118.96	0.4107
25	131.61	1.0825

26	134.99	0.6933
27	144.41	2.4505

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**Au<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.77	0.0000
2	19.81	0.0305
3	20.45	0.0000
4	26.28	0.0001
5	28.79	0.4316
6	28.85	0.0510
7	40.14	0.0017
8	40.27	0.1719
9	43.22	0.0000
10	45.82	0.9524
11	46.28	0.4135
12	47.5	0.1719
13	52.49	0.5716
14	52.57	0.0768
15	56.7	0.0000
16	57.63	0.0010
17	62.23	0.0800
18	65.44	0.1333
19	68.24	1.2112
20	77.18	0.2512
21	83.39	0.0002
22	86.04	0.0066
23	89.81	0.5515
24	90.12	0.0266
25	98.42	0.7600
26	101.53	3.0654
27	131.17	0.5672
28	136.64	0.7892
29	141.49	6.3020
30	148.02	6.0451

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**Au<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.51	0.0000
2	18.2	0.2606
3	24.36	0.0227
4	26.54	0.0000
5	27.78	0.0160
6	32.4	0.0023
7	38.15	0.0152
8	39.32	0.0000

9	40.67	0.4442
10	42.3	0.1857
11	42.7	0.5787
12	44.92	0.0000
13	49.65	0.3390
14	51.05	0.0903
15	53.73	0.0134
16	53.94	0.0809
17	54.4	0.0286
18	57.2	0.0064
19	61.38	0.0538
20	62.58	0.2476
21	67.2	0.7502
22	73.24	0.0391
23	75.37	0.0000
24	82.21	0.0400
25	84.22	0.7214
26	85.56	0.0215
27	94.54	0.0971
28	95.56	0.0335
29	99.8	3.0523
30	118.37	0.1062
31	127.62	0.4275
32	139.28	4.3771
33	145.2	4.6817

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**Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.39	0.0009
2	14.59	0.0668
3	16.51	0.0045
4	25.39	0.0021
5	29.01	0.0000
6	34.67	0.0245
7	34.74	0.1900
8	34.99	0.0073
9	36.45	0.0001
10	43.49	0.1418
11	46.41	0.0004
12	47.5	0.0005
13	48.77	0.4690
14	48.77	0.3389
15	49.15	0.3382
16	50.47	0.0063
17	55.78	0.1451

18	58.36	0.0009
19	59.81	0.3488
20	60.47	0.7098
21	63.09	0.0406
22	66.14	0.0454
23	68.8	0.0342
24	71.33	0.2368
25	87.73	0.0176
26	89.43	0.1333
27	91.01	0.9893
28	93.94	0.2211
29	95.9	1.6269
30	99.78	0.0001
31	101.94	0.0507
32	114.38	0.1433
33	117.79	1.6855
34	122.3	2.6633
35	135.7	0.2906
36	140.97	0.0159

**Au<sub>15</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.23	0.0264
2	24.43	0.0268
3	27.24	0.0001
4	27.54	0.0000
5	29.43	0.0000
6	33.88	0.0290
7	35.21	0.0832
8	36.78	0.0000
9	37.61	0.0406
10	43.14	0.0076
11	44.06	0.0469
12	47.58	0.1964
13	47.7	0.0391
14	48.88	0.0000
15	50.22	0.0000
16	53	1.6501
17	55.24	0.1551
18	56.51	0.0219
19	56.72	0.0008
20	59.22	0.0000
21	59.91	0.2323
22	60.21	0.0269
23	61.82	0.0252



24	63.68	0.0195
25	65.86	0.0000
26	66.58	0.1226
27	78.38	0.4360
28	83.49	0.3354
29	84.57	0.0099
30	90.42	0.0212
31	91.43	0.0000
32	93.9	0.1289
33	94.77	0.0232
34	97.65	0.3543
35	102.59	0.8412
36	107.8	1.4670
37	113.73	0.2159
38	119.93	0.2953
39	126.81	0.0444

**Au<sub>16</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.72	0.0562
2	19.13	0.0210
3	22.26	0.0075
4	24.73	0.0115
5	25.67	0.0009
6	27.77	0.0129
7	28.86	0.0280
8	31.17	0.1256
9	35.22	0.0730
10	37.78	0.0157
11	40.14	0.2398
12	40.63	0.0258
13	41.5	0.0710
14	44.03	0.0370
15	46.99	0.1164
16	47.76	0.0400
17	48.31	0.1149
18	51.18	0.4363
19	54.24	0.1164
20	55.25	0.1370
21	56.67	0.0717
22	58.58	0.4082
23	60.17	0.2497
24	61.75	0.2401
25	62.08	0.0137
26	66	0.2783

27	70.97	0.0441
28	71.34	0.0602
29	78.76	0.1311
30	82.84	0.0757
31	87.76	0.1701
32	90.39	0.2417
33	91.98	0.0840
34	94.29	0.9549
35	99.25	0.0307
36	101.63	0.9634
37	102.38	0.2581
38	108.25	0.4320
39	118.74	1.3402
40	124.77	3.4946
41	128.45	0.8810
42	142.87	0.1829

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**Au<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.41	0.0054
2	20.94	0.0000
3	21.24	0.1236
4	31.39	0.0161
5	31.4	0.0055
6	33.41	0.1419
7	33.68	0.0783
8	35.66	0.0025
9	37.19	0.1847
10	38	0.1310
11	38.97	0.0000
12	41.21	0.0048
13	43.47	0.0320
14	47.03	0.1107
15	50.33	0.0000
16	51.38	0.0658
17	52.94	0.0000
18	53.2	0.0132
19	54.25	0.0485
20	55.68	0.0431
21	58.15	0.9977
22	59	0.0158
23	59.69	0.0611
24	60.08	0.2570
25	61.27	0.0000
26	61.98	0.4661

27	64.76	0.0432
28	68.12	0.0004
29	68.41	0.8525
30	82.62	0.3913
31	85.39	0.0000
32	85.48	0.0072
33	86.13	0.0086
34	88.16	0.0428
35	91.39	0.0000
36	96.24	0.0695
37	98.61	0.2506
38	98.81	0.1437
39	102.34	0.0299
40	104.57	0.0000
41	105.37	0.1216
42	107.61	1.3804
43	111.95	1.0997
44	113.88	0.0020
45	120.51	0.0851

**Au<sub>18</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.43	0.2042
2	23.77	0.0237
3	27.47	0.0022
4	27.78	0.0915
5	29.54	0.2144
6	30.44	0.0000
7	31.81	0.1723
8	33.75	0.0356
9	33.88	0.0002
10	36.54	0.0116
11	37.24	0.1891
12	37.42	0.0081
13	39.51	0.0765
14	43.66	0.0628
15	44.27	0.0173
16	45.92	0.0730
17	47.25	0.1968
18	48.27	0.1536
19	50.66	0.2029
20	52.53	0.0113
21	54.28	0.0269
22	56.56	0.2434
23	58.35	0.4699

24	58.98	0.0301
25	59.16	0.0392
26	60.37	0.1150
27	63.24	0.0171
28	63.84	0.6232
29	64.51	0.1190
30	69.99	0.1024
31	72.47	0.0847
32	76.62	0.0198
33	82.04	0.1465
34	87.55	0.0020
35	89.9	0.0194
36	91.33	0.0475
37	93.34	0.0021
38	94.95	0.0434
39	96.29	0.0028
40	98.45	0.0089
41	100.7	0.0169
42	105.07	0.2656
43	107.81	0.1806
44	109.37	0.0050
45	111.28	0.1288
46	116.31	0.9455
47	119.08	0.3577
48	122.02	1.2551

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**Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	28.15	0.0047
2	28.47	0.0036
3	28.71	0.0003
4	29.77	0.1201
5	31.91	0.2534
6	32.2	0.2759
7	33.59	0.0007
8	33.97	0.0080
9	39.84	0.0506
10	40.09	0.0937
11	40.48	0.0648
12	43.11	0.0529
13	43.5	0.1028
14	44.21	0.1568
15	44.5	0.1186
16	44.69	0.1412
17	46.98	0.0016

18	49.59	0.4530
19	49.76	0.5794
20	49.84	0.6551
21	52.3	0.4956
22	52.77	0.0169
23	53.01	0.0341
24	55.51	0.0001
25	55.86	0.0007
26	56.47	0.0011
27	59.87	0.0022
28	59.95	0.0036
29	60.86	0.2132
30	62.76	0.0003
31	64.66	0.0840
32	64.88	0.0768
33	72.72	0.0000
34	77.6	0.0224
35	83.07	0.2699
36	85.49	0.0913
37	85.7	0.0949
38	87.29	0.0005
39	90.31	0.0760
40	90.38	0.0996
41	94.61	0.1468
42	94.78	0.1252
43	99.41	0.3615
44	105.35	5.2164
45	105.43	5.2120
46	124.99	1.7035
47	125.12	1.7258
48	125.86	3.4366
49	141.68	0.1724
50	141.79	0.1655
51	147.26	0.0743

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**Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	28.5	0.0000
2	28.5	0.0000
3	28.52	0.0000
4	31.93	0.2524
5	32.61	0.2508
6	32.61	0.2508
7	34.37	0.0000
8	34.55	0.0000

9	41.17	0.0000
10	41.6	0.0272
11	41.89	0.0000
12	42.1	0.0266
13	42.1	0.0266
14	45.95	0.0014
15	45.95	0.0014
16	46.49	0.0000
17	48.42	0.0000
18	50.84	1.2641
19	51.27	1.2657
20	51.27	1.2657
21	51.59	0.0000
22	52.38	0.0000
23	54.17	0.0000
24	56.22	0.0014
25	56.22	0.0014
26	56.88	0.0000
27	58.47	0.1082
28	59	0.0779
29	59	0.0779
30	62.08	0.0406
31	62.3	0.0472
32	62.3	0.0472
33	72.2	0.0000
34	72.2	0.0000
35	72.61	0.0000
36	74.02	0.0000
37	79.43	0.0000
38	88.03	0.0000
39	88.07	0.0001
40	88.07	0.0001
41	90.63	0.0000
42	91.44	0.0000
43	96.37	0.0684
44	96.59	0.0814
45	96.59	0.0814
46	107.79	8.9651
47	107.87	8.9803
48	107.87	8.9803
49	138.29	0.0000
50	138.47	0.0000
51	143.83	0.1754
52	143.91	0.1697
53	143.91	0.1697

54	149.74	0.0000
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**CH<sub>4</sub>\_Au<sub>1</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	77.97	2.0458
2	134.04	0.0143
3	145.51	0.0138
4	1385.38	89.4361
5	1394.36	37.2971
6	1394.43	37.6643
7	1588.22	1.8871
8	1588.76	1.9874
9	3052.37	3.2368
10	3186.7	25.4756
11	3186.96	25.3510
12	3195.52	57.9571

**CH<sub>4</sub>\_Au<sub>2</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.27	0.1258
2	32.8	0.5969
3	63.88	0.6833
4	127.03	11.1614
5	173.73	10.2775
6	184.38	0.0092
7	1341.89	20.9929
8	1387.04	46.4785
9	1417.31	57.2042
10	1581.97	0.0790
11	1583.63	38.7726
12	3006.37	94.2494
13	3104.3	9.8073
14	3168.98	99.4300
15	3221.71	12.1745

**CH<sub>4</sub>\_Au<sub>3</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.45	0.2533
2	23.17	0.1443
3	41.05	0.0068
4	44.61	1.4075
5	56.95	0.6502
6	77.26	4.8061
7	123.98	2.3549
8	157.44	15.8767
9	216.37	0.1673
10	1338.35	22.0684

11	1388.16	39.8096
12	1423.04	44.4191
13	1581.82	0.3071
14	1585.09	31.5057
15	2999.67	88.0352
16	3092.64	35.2318
17	3167.62	76.0860
18	3223.09	10.3126

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**CH<sub>4</sub> Au<sub>4</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.75	0.1231
2	27.75	0.2545
3	36.65	0.2861
4	39.41	0.0000
5	58.46	0.1386
6	59.02	3.7131
7	81.5	0.0042
8	92.79	0.0646
9	127.01	10.2863
10	133.39	2.1040
11	168.64	13.1147
12	280.84	0.0075
13	1328.03	16.3865
14	1391.3	36.2674
15	1426.52	52.9570
16	1578.62	0.0000
17	1590.85	28.8134
18	2999.34	85.6936
19	3092.07	13.6422
20	3168.83	69.5387
21	3225.91	6.2877

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**CH<sub>4</sub> Au<sub>5</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	22.09	0.0000
2	24.19	0.0108
3	27.38	0.0020
4	29.41	0.0364
5	48.88	0.1746
6	57.46	0.1764
7	66.96	0.0018
8	77.6	0.2652
9	86.26	0.1105
10	91.03	0.8151
11	100.66	0.0856



12	107.08	0.0373
13	116.65	0.2785
14	119.41	0.5793
15	147.16	4.7751
16	1379.38	67.4500
17	1387.11	22.4482
18	1387.95	23.2446
19	1580.57	4.0144
20	1580.81	5.7769
21	3046.12	1.0609
22	3178.38	17.8693
23	3179.25	20.6219
24	3192.61	60.0967

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**CH<sub>4</sub> Au<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	27.59	0.0006
2	27.91	0.0003
3	30.46	0.0007
4	31.38	0.0002
5	32.24	0.0989
6	53.22	0.1827
7	53.48	0.1755
8	71.03	0.6643
9	71.15	0.6622
10	84.8	0.0054
11	94.03	0.1541
12	98.78	0.5368
13	104.19	0.0537
14	112.27	0.0001
15	136.79	0.4047
16	153.25	5.2214
17	155.31	9.4476
18	156.55	4.6089
19	1385.94	51.6367
20	1389.31	30.1510
21	1389.57	23.3560
22	1583.8	2.6745
23	1585.87	2.7869
24	3045.42	0.7494
25	3177.71	24.7604
26	3178.47	24.7123
27	3190.5	58.8927

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**CH<sub>4</sub> Au<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
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1	10.79	0.0057
2	15.55	0.1121
3	25.92	0.0005
4	27.32	0.0002
5	30.6	0.0871
6	32.82	0.0012
7	36.4	0.0032
8	45.82	0.0298
9	53.8	0.3148
10	67.6	0.3418
11	72.9	0.1716
12	88.09	0.1556
13	91.7	0.0073
14	95.2	0.1452
15	98.02	0.0593
16	101.03	0.6571
17	127.51	1.9091
18	129.34	0.3347
19	143.59	6.8670
20	148.7	0.4226
21	158.8	5.9416
22	1383.32	43.1310
23	1387.63	31.3757
24	1388.57	20.4561
25	1582.5	2.8539
26	1584.36	2.5702
27	3043.8	0.6318
28	3173.96	23.4176
29	3178.04	21.3442
30	3189.85	53.7711

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**CH<sub>4</sub> Au<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.23	0.0000
2	22.33	0.0000
3	29.31	0.0656
4	30.34	0.1950
5	32.19	0.0096
6	34.88	0.0179
7	36.49	0.0003
8	38.76	0.0365
9	46.62	0.0015
10	53.91	0.2107
11	54.27	0.2268
12	65.13	0.0009

13	73.12	0.0001
14	77.29	0.0115
15	90.32	1.2239
16	90.36	1.2128
17	100.95	0.5925
18	104.03	0.0719
19	109	0.0639
20	115.61	0.0245
21	116.43	0.0014
22	153.55	15.4196
23	153.95	15.3426
24	170.73	0.0098
25	1376.16	54.1847
26	1384.23	18.0823
27	1385.41	17.4431
28	1576.16	0.6131
29	1581.8	0.6888
30	3040.23	1.3562
31	3164.25	36.1143
32	3179.02	23.1114
33	3189.06	46.7787

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**CH<sub>4</sub>\_Au<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.79	0.0000
2	11.53	0.0124
3	22.91	0.0059
4	26.67	0.0163
5	29.68	0.0671
6	30.56	0.0691
7	32.14	0.0008
8	34.16	0.0023
9	37.2	0.0079
10	42.36	0.0076
11	45.17	0.0138
12	47.64	0.0043
13	64.04	0.0002
14	66.52	0.0018
15	67.25	0.0163
16	69.26	0.1087
17	82.03	0.1515
18	82.3	1.1869
19	92.07	0.0358
20	105.8	0.6649
21	107.58	0.0008

22	119.05	0.2246
23	131.12	0.1206
24	144.06	9.1672
25	144.12	7.5669
26	157.91	0.4137
27	159.53	1.0071
28	1380.57	46.2291
29	1383.6	17.4877
30	1388.43	21.0124
31	1579.81	1.6085
32	1581.89	2.2987
33	3040.35	0.9299
34	3168.45	20.8624
35	3174.55	18.2862
36	3187.88	48.0041

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**CH<sub>4</sub>-Au<sub>10</sub>**

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Mode	Frequency	Infrared
1	13.15	0.0023
2	11.32	0.0001
3	13.59	0.0179
4	18.02	0.0018
5	21.56	0.0002
6	24.67	0.0112
7	27.66	0.0013
8	31.5	0.0593
9	37.69	0.0087
10	43.38	0.0002
11	44.69	0.0944
12	49.09	0.0002
13	53.2	0.0070
14	58.42	0.0672
15	67.35	0.3291
16	67.39	1.2239
17	68.51	0.0012
18	73.2	0.0050
19	77.54	0.0000
20	86.29	0.0109
21	87.25	0.0001
22	99.06	0.0000
23	105.51	0.4396
24	107.56	0.6210
25	116.23	3.1636
26	132.85	0.0102
27	133.05	3.7406

28	134.54	0.0001
29	146.29	0.0848
30	163.33	0.0042
31	1379.54	44.5163
32	1385.94	16.7798
33	1386.78	19.1942
34	1578.72	4.1732
35	1582.6	4.1574
36	3040.53	1.1188
37	3166.69	10.6615
38	3175.62	14.1860
39	3188.1	51.0831

---

**CH<sub>4</sub> Au<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.54	0.0005
2	10.98	0.0009
3	13.87	0.0152
4	16.1	0.0037
5	20.72	0.0305
6	23.46	0.0010
7	26.93	0.0330
8	27.92	0.0066
9	31.19	0.0075
10	36.21	0.0075
11	42.32	0.0578
12	42.43	0.0243
13	46.17	0.0463
14	48.83	0.0919
15	53.86	0.2514
16	55.93	0.0591
17	59.88	0.0467
18	62.99	0.0772
19	71.92	0.0794
20	74.07	0.4409
21	79.76	0.6457
22	83.53	0.0624
23	87.53	0.1883
24	99.97	0.1770
25	105.44	0.2082
26	107.28	0.4102
27	111.67	3.4923
28	119.34	0.4901
29	131.81	0.9603
30	133.73	0.5783

31	136.4	0.2074
32	144.97	2.5512
33	156.37	0.0635
34	1382.24	41.8420
35	1384.95	20.4644
36	1386.64	17.1058
37	1579.7	3.3917
38	1582.5	4.6518
39	3041.08	0.7597
40	3168.98	12.1998
41	3173.83	11.6716
42	3187.56	50.2554

---

**CH<sub>4</sub> Au<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.69	0.0009
2	19.13	0.0924
3	20.6	0.0007
4	24.25	0.0051
5	28.21	0.0054
6	30.7	0.0641
7	32.29	0.1544
8	34.04	0.3064
9	37.53	0.3483
10	41.63	0.2245
11	41.83	0.1769
12	42.69	0.0044
13	46.82	0.0693
14	47.85	0.4318
15	52.38	0.1059
16	53.12	0.7710
17	56.34	0.0029
18	57.37	0.0944
19	62.16	0.0868
20	62.54	0.0761
21	64.98	0.2126
22	67.55	1.0652
23	76.79	0.1835
24	84.39	0.0115
25	87.12	0.0579
26	89.77	0.9176
27	91	0.0388
28	97.85	1.3945
29	101.5	3.1918
30	104.62	0.5433

31	113.74	0.0533
32	131.92	0.6694
33	134.15	0.0155
34	137.31	1.0070
35	140.85	5.9506
36	147.4	5.9873
37	1373.53	71.7742
38	1383.33	16.0641
39	1384.01	16.9415
40	1575	7.1283
41	1578.4	2.3902
42	3037.82	4.4506
43	3161.68	19.6834
44	3169.65	12.1784
45	3188.49	68.1254

---

**CH<sub>4</sub> Au<sub>13</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.78	0.0100
2	18.63	0.2210
3	20.08	0.0224
4	23.26	0.0025
5	25.99	0.0162
6	27.56	0.0182
7	27.78	0.0343
8	32.62	0.0036
9	37.47	0.0171
10	39.33	0.0002
11	40.93	0.3804
12	42.36	0.1365
13	43.69	0.7175
14	44.62	0.0072
15	48.93	0.4321
16	50.88	0.0901
17	52.79	0.0551
18	53.19	0.0252
19	53.73	0.0051
20	56.94	0.0032
21	61.29	0.0543
22	62.39	0.2545
23	64.53	0.0319
24	67.05	0.7584
25	73.23	0.0441
26	74.73	0.0410
27	81.63	0.1280

28	83.93	0.6967
29	85.44	0.0455
30	94.25	0.1404
31	94.9	0.3240
32	97.75	0.9461
33	99.68	3.5308
34	118.48	0.0777
35	127.63	0.4646
36	133.8	0.2049
37	139.38	4.3942
38	144.48	1.2832
39	145.59	3.3514
40	1379.4	93.5606
41	1383.22	17.3767
42	1387.58	15.4898
43	1580.11	4.7618
44	1581.77	6.0997
45	3041.42	2.4854
46	3168.99	13.9696
47	3173.94	13.4499
48	3189.19	84.3756

---

**CH<sub>4</sub>\_Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.16	0.0241
2	11.36	0.0434
3	14.81	0.0172
4	17.31	0.0670
5	22.45	0.0435
6	25.29	0.0167
7	28.98	0.0018
8	34.31	0.0021
9	34.65	0.0627
10	35.61	0.1226
11	36.84	0.0096
12	43.19	0.0896
13	45.54	0.0229
14	46.91	0.0026
15	47.63	0.0776
16	48.04	0.2566
17	49.41	0.4136
18	50.58	0.2737
19	51.14	0.1557
20	55.83	0.1522
21	57.6	0.4932



22	58.48	0.1823
23	60.63	0.6330
24	63.29	0.0352
25	65.78	0.0411
26	68.7	0.0575
27	70.46	0.2464
28	87.74	0.0688
29	89.15	0.1157
30	91.24	0.8337
31	94.56	0.8393
32	95.86	1.0551
33	98.2	0.7588
34	101.03	0.1019
35	106.55	1.9676
36	113.63	1.4522
37	114.74	0.7007
38	118.01	1.9780
39	122.22	2.5414
40	137.23	0.0544
41	141.97	0.2627
42	175.9	0.3041
43	1378.52	99.2773
44	1384.1	40.8919
45	1392.08	20.0367
46	1578.42	6.5502
47	1586.19	6.0954
48	3039.62	9.0779
49	3161.03	15.2537
50	3174.47	31.5342
51	3189.98	66.6866

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**CH<sub>4</sub>-Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.31	0.0208
2	17.15	0.0337
3	23.71	0.0209
4	24.53	0.0157
5	26.15	0.0026
6	27.2	0.0001
7	28.33	0.0142
8	33.17	0.0425
9	35.04	0.0712
10	36.99	0.0105
11	38.1	0.0389
12	43.33	0.0022

13	44.44	0.0528
14	47.31	0.1911
15	47.53	0.0681
16	48.82	0.0033
17	49.55	0.0045
18	53.7	1.4794
19	54.54	0.1689
20	56.17	0.0345
21	56.84	0.0292
22	57.35	0.0575
23	58.63	0.0566
24	59.43	0.2622
25	60.54	0.0285
26	61.61	0.0222
27	63.07	0.0229
28	64.64	0.0015
29	66.61	0.1206
30	78.05	0.4358
31	82.79	0.3444
32	84.29	0.0175
33	89.93	0.0274
34	90.74	0.0064
35	93.48	0.1052
36	94.58	0.0636
37	97.49	0.2860
38	102.27	0.8872
39	105.91	2.3822
40	107.78	1.7655
41	113.62	0.2294
42	117.76	0.7240
43	121.85	0.1167
44	127.67	0.2511
45	136.83	0.0559
46	1380.31	108.1549
47	1384.69	19.8131
48	1388.49	17.2461
49	1580.53	5.9934
50	1584.02	6.8907
51	3041.39	4.2832
52	3167.89	13.8368
53	3172.97	15.6707
54	3185.34	74.2412

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**CH<sub>4</sub> Au<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
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1	10.38	0.0063
2	15.37	0.0734
3	18.48	0.0125
4	20.03	0.0351
5	22.59	0.0092
6	24.93	0.0137
7	25.3	0.0128
8	27.22	0.0153
9	29.32	0.0273
10	30.56	0.1554
11	35.28	0.0950
12	37.75	0.0082
13	39.7	0.1838
14	40.54	0.0232
15	41.88	0.1283
16	43.96	0.0244
17	46.66	0.0825
18	47.68	0.0582
19	48.3	0.1143
20	51.75	0.4355
21	53.62	0.1180
22	55.01	0.1395
23	56.56	0.1033
24	57.98	0.0632
25	58.67	0.2828
26	60.17	0.2057
27	62.11	0.2479
28	62.36	0.1581
29	66.11	0.2363
30	70.22	0.0238
31	71.61	0.0599
32	78.7	0.1815
33	82.78	0.0787
34	87.65	0.1778
35	89.81	0.1200
36	91.78	0.1004
37	93.98	0.8649
38	98.54	0.3598
39	101.1	1.1045
40	102.45	0.5425
41	107.9	0.4488
42	110.9	1.8697
43	117.52	1.7669
44	118.9	0.3329
45	125.16	3.4487

46	129.08	0.8038
47	143.74	0.2112
48	149.58	0.1873
49	1381.79	97.3561
50	1383.59	17.2536
51	1388.19	16.4534
52	1578.91	5.6051
53	1584.11	6.3374
54	3040.78	3.8148
55	3163.66	16.5239
56	3175.91	11.6987
57	3186.15	68.0096

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**CH<sub>4</sub> Au<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.85	0.0575
2	15.48	0.0047
3	20.25	0.0163
4	20.94	0.1033
5	22.19	0.2422
6	30.9	0.0023
7	31.2	0.0139
8	33.15	0.0838
9	34.02	0.1543
10	35.15	0.0017
11	37.39	0.1843
12	37.72	0.1043
13	38.01	0.0083
14	41.42	0.0150
15	43.39	0.0369
16	43.56	0.0161
17	46.77	0.1128
18	50.64	0.0019
19	50.88	0.0502
20	53.1	0.0015
21	53.57	0.0135
22	53.91	0.0667
23	54.02	0.0481
24	58.45	0.8493
25	59.28	0.0071
26	59.64	0.2942
27	59.99	0.1450
28	60.21	0.0136
29	62.17	0.6950
30	63.86	0.0367

31	66.48	0.0057
32	67.85	0.8476
33	81.31	0.4217
34	82.85	0.7101
35	85.84	0.0192
36	85.87	0.0013
37	87.98	0.2120
38	89.54	0.0000
39	96.07	0.1111
40	97.15	0.9538
41	98.92	0.7550
42	101.45	2.3811
43	102.15	0.3662
44	104.53	0.0349
45	104.99	0.1177
46	107.83	1.5251
47	112.61	0.3462
48	114.46	0.0033
49	121.34	0.1639
50	138.72	0.2697
51	156.13	0.0870
52	1374.65	117.6083
53	1383.86	34.1516
54	1392.55	15.0170
55	1579.8	4.6120
56	1582.88	6.7580
57	3039.63	5.8661
58	3163.01	14.9056
59	3174.46	16.8119
60	3189.81	88.2124

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**CH<sub>4</sub>-Au<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	1.05	0.0459
2	12.85	0.0270
3	20.14	0.2193
4	23.6	0.0188
5	26.81	0.0053
6	27.51	0.0875
7	29.21	0.1630
8	30.32	0.0148
9	31.82	0.1947
10	33.27	0.0271
11	33.81	0.0029
12	36.19	0.0082

13	36.8	0.1133
14	37.22	0.0995
15	39.22	0.0996
16	43.61	0.0239
17	43.83	0.0394
18	45.59	0.0446
19	45.68	0.0341
20	46.94	0.3253
21	47.92	0.1244
22	50.73	0.1987
23	52.12	0.0024
24	53.66	0.0482
25	56.46	0.2180
26	57.8	0.1398
27	58.42	0.2693
28	58.86	0.0857
29	59.88	0.1344
30	63.09	0.6731
31	63.6	0.1419
32	63.8	0.0208
33	69.29	0.1500
34	71.41	0.1194
35	76.58	0.0212
36	81.72	0.1700
37	85.77	1.1561
38	89.11	0.4342
39	90.11	0.4292
40	92.71	0.2695
41	94.42	0.3163
42	96.24	0.1141
43	97.42	0.7456
44	100.43	1.4651
45	101.2	1.0705
46	104.95	0.1063
47	107.54	0.3927
48	109.75	0.0773
49	112.09	0.4102
50	117.42	0.3935
51	118.56	0.3385
52	122.69	1.2332
53	132.1	0.3201
54	149.15	0.1148
55	1373.98	149.6878
56	1385.51	24.2045
57	1388.17	20.4616

58	1578.84	5.4690
59	1579.8	5.9011
60	3038.88	12.7148
61	3162.84	16.3318
62	3171.92	14.4726
63	3188.73	108.8920

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**CH<sub>4</sub>\_Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	27.1	0.0021
2	2.95	0.0118
3	12.05	0.0118
4	28.71	0.0029
5	29.36	0.0089
6	29.62	0.0017
7	30.01	0.0627
8	33.29	0.2957
9	33.51	0.2828
10	34.03	0.0034
11	34.1	0.0004
12	40.69	0.0467
13	40.76	0.0473
14	41.09	0.0475
15	43.66	0.1108
16	43.83	0.1018
17	44.96	0.1780
18	45.2	0.0177
19	45.72	0.1854
20	47.39	0.0004
21	50.09	0.6986
22	50.2	0.6492
23	50.34	0.6869
24	52.66	0.2603
25	53.4	0.0357
26	53.67	0.0253
27	55.5	0.0015
28	56.22	0.0010
29	56.81	0.0003
30	60	0.0026
31	60.33	0.0055
32	61.35	0.2298
33	62.88	0.0003
34	64.95	0.0721
35	65.29	0.0694
36	73.49	0.0000

37	77.84	0.0086
38	82.99	0.2519
39	85.87	0.0680
40	85.94	0.0704
41	87.32	0.0002
42	90.53	0.1028
43	90.71	0.0839
44	94.85	0.1477
45	95.05	0.1504
46	99.64	0.5692
47	105.24	4.6030
48	105.41	5.3074
49	106.43	2.4933
50	124.61	1.7026
51	124.81	1.7009
52	125.8	3.3734
53	133.03	0.1387
54	141.98	0.1437
55	142.17	0.1317
56	147.5	0.0657
57	158.29	0.0062
58	1381.79	73.4388
59	1383.3	15.3725
60	1385	13.6448
61	1580.57	5.7645
62	1582.24	5.8979
63	3041.03	0.6851
64	3169.96	8.4348
65	3172.9	10.3010
66	3184.12	71.3993

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**CH<sub>4</sub>-Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.4	0.0141
2	24.96	0.0024
3	28.39	0.0013
4	28.66	0.0010
5	31.24	0.0441
6	31.53	0.2346
7	31.89	0.1608
8	32.19	0.2288
9	34.18	0.0020
10	34.41	0.0090
11	41.4	0.0150
12	41.54	0.0269



13	41.68	0.0302
14	41.8	0.0237
15	41.95	0.0272
16	46.02	0.0005
17	46.18	0.0035
18	46.55	0.0008
19	48.57	0.0005
20	50.93	1.2193
21	51.04	1.3544
22	51.23	1.2327
23	52	0.0322
24	52.18	0.0302
25	53.45	0.0005
26	56.15	0.0030
27	56.35	0.0015
28	56.71	0.0072
29	58.58	0.0961
30	58.69	0.0622
31	58.87	0.0774
32	61.98	0.0732
33	62.09	0.0453
34	62.38	0.0441
35	71.42	0.0007
36	72.29	0.0049
37	72.38	0.0005
38	72.49	0.0002
39	73.94	0.0002
40	79.4	0.0001
41	87.34	0.0461
42	87.78	0.0053
43	88.08	0.0010
44	90.66	0.0037
45	91.2	0.0093
46	96.19	0.0106
47	96.39	0.0633
48	96.67	0.1232
49	103.83	2.7451
50	107.74	9.0531
51	107.78	8.8556
52	108.19	8.2888
53	138.59	0.0026
54	138.68	0.0056
55	140.82	0.0017
56	144.05	0.1723
57	144.09	0.1579

58	144.29	0.1828
59	149.96	0.0005
60	153.93	0.0201
61	1379.53	66.5695
62	1382.08	24.8840
63	1385.92	14.9585
64	1578.8	4.2121
65	1580.28	4.4813
66	3039.72	1.4162
67	3167.73	9.9217
68	3170.74	12.1107
69	3185.02	81.0796

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**CO\_Au<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	160	21.9052
2	256.05	25.2545
3	1992.43	1241.7325

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**CO\_Au<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	44.62	0.0170
2	164.71	3.7965
3	280.55	9.3205
4	298.07	10.8623
5	310.57	1.1395
6	2137.89	631.9650

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**CO\_Au<sub>3</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.6	0.2520
2	48.85	0.0136
3	72.01	1.1014
4	81.81	0.1603
5	138.8	5.5423
6	283.4	0.0108
7	302.48	6.3846
8	342.27	12.2128
9	2103.73	1493.2523

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**CO\_Au<sub>4</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	26.97	0.0200
2	29.42	0.1910
3	51.33	0.0069
4	56.15	2.1026
5	63.06	0.3705
6	86.18	0.3236

7	138.68	9.2181
8	140.75	0.7130
9	296.38	5.7634
10	305.51	0.0059
11	338.79	8.9111
12	2115.5	1007.7676

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**CO\_Au<sub>5</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.65	0.0247
2	18.2	0.0327
3	25.75	0.0505
4	29.99	0.0581
5	48.95	0.1907
6	57.71	0.1952
7	63.35	0.0588
8	65.49	0.1697
9	77.86	0.3542
10	86.81	0.1245
11	106.24	0.1468
12	114.5	1.8080
13	119.66	0.4957
14	147.92	4.7688
15	2091.03	71.0730

---

**CO\_Au<sub>6</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.34	0.0554
2	20.61	0.0082
3	28.23	0.0005
4	30.14	0.0138
5	30.88	0.1363
6	48.5	0.1462
7	54.25	0.1777
8	55.32	0.1559
9	62.45	0.0031
10	71.47	0.6337
11	72.03	0.6703
12	94.81	0.0077
13	103.22	0.0280
14	111.05	0.2413
15	113.63	0.0030
16	154.99	9.5701
17	156.49	9.3052
18	2092.46	78.7621

---

**CO\_Au<sub>7</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.91	0.1311
2	10.51	0.0221
3	17.94	0.0671
4	19.85	0.0378
5	27.27	0.0641
6	27.62	0.0015
7	30.53	0.1160
8	44.94	0.0409
9	45.65	0.0426
10	53.78	0.3079
11	66.07	0.0770
12	68.08	0.3777
13	72.71	0.1467
14	84.3	0.1633
15	93.69	0.1682
16	95.61	0.0931
17	98.15	0.0553
18	127.1	1.7820
19	143.1	6.6922
20	158.51	6.2233
21	2095.96	106.9569

**CO\_Au<sub>8</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.19	0.0006
2	12.3	0.0499
3	15.06	0.0550
4	21.62	0.0002
5	29.48	0.2346
6	33.38	0.0150
7	33.49	0.0175
8	35.37	0.0001
9	46.37	0.0001
10	53.25	0.2689
11	53.38	0.2663
12	72.73	0.0000
13	73.32	0.0057
14	86.53	0.1860
15	89.85	1.5564
16	90.24	1.2755
17	90.59	0.0851
18	92.95	0.1854
19	108.78	0.0135
20	115.92	0.0001

21	153.27	15.6430
22	153.34	15.6314
23	170.24	0.0000
24	2098.36	212.4548

---

**CO\_Au<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	3.97	0.0108
2	9.57	0.0162
3	14.62	0.0582
4	20.54	0.0901
5	26.26	0.0981
6	29.5	0.6361
7	32.4	0.2537
8	34.89	0.0029
9	40.04	0.0823
10	42.74	0.0557
11	48.92	0.0442
12	50.59	0.0240
13	58.21	0.1693
14	62.06	1.4528
15	66.45	0.0380
16	79.24	0.5439
17	86.43	0.6955
18	91.96	1.6743
19	99.5	0.1584
20	107.34	0.9147
21	124.69	0.3500
22	147.61	9.6479
23	163.63	5.9794
24	232.86	0.9831
25	252.92	0.3571
26	263.6	3.6741
27	2106.09	564.1113

---

**CO\_Au<sub>10</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.97	0.0013
2	10.89	0.0027
3	17.19	0.1030
4	17.64	0.0276
5	21.83	0.0015
6	25.91	0.0185
7	29.19	0.0042
8	29.44	0.0018
9	36.09	0.0744

10	43.57	0.0000
11	44.63	0.0976
12	48.76	0.0007
13	58.34	0.0796
14	66.78	0.3374
15	67.12	1.2057
16	68.18	0.0126
17	69.04	0.1394
18	73.12	0.0049
19	77.14	0.0016
20	85.47	0.0421
21	87.31	0.0016
22	94.52	0.0099
23	98.88	0.0005
24	104.91	0.4773
25	113.78	0.3840
26	115.99	3.2849
27	131.94	3.0382
28	132.25	0.0200
29	134.2	0.6516
30	2096.52	143.8234

---

**CO\_Au<sub>11</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.93	0.0033
2	10.55	0.0141
3	11.43	0.0199
4	15.1	0.0500
5	18.44	0.0239
6	21.24	0.0529
7	26.61	0.0382
8	28.42	0.0090
9	30.86	0.0137
10	36.24	0.0084
11	41.24	0.0177
12	42.18	0.0306
13	43.59	0.1380
14	46.5	0.0649
15	49.02	0.0770
16	54.4	0.2690
17	58.75	0.2869
18	59.83	0.1673
19	63.09	0.0757
20	71.85	0.0737
21	74.48	0.4510

22	80.12	0.6138
23	83.93	0.0674
24	87.31	0.2094
25	96.93	0.0157
26	100.15	0.1785
27	106.36	0.0512
28	111.7	3.5247
29	118.94	0.4442
30	131.9	1.0503
31	135.24	0.7022
32	145.35	2.5735
33	2091.63	62.8489

---

**CO\_Au<sub>12</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.77	0.0230
2	11.73	0.0556
3	19	0.0408
4	19.68	0.1258
5	23.52	0.0210
6	26.83	0.1986
7	30.27	0.0405
8	30.58	0.0242
9	32.99	0.2905
10	34.51	0.1079
11	41.15	0.0087
12	42.56	0.1344
13	46.6	0.1401
14	50	0.0446
15	51.67	0.2808
16	55.55	0.2559
17	57.69	0.5012
18	61.98	0.2955
19	64.89	0.2453
20	68.26	0.8818
21	72.23	0.5698
22	77.85	0.0896
23	83.98	0.2102
24	87.78	0.0166
25	94.2	0.6775
26	98.16	0.4980
27	102.21	1.9754
28	110.99	2.8172
29	134.35	2.5118
30	141.1	5.5721

31	148.71	1.0604
32	151.74	6.9838
33	240.96	9.0247
34	260.07	10.0748
35	266.12	4.3404
36	2134.14	588.9439

---

**CO Au<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.48	0.0325
2	11.5	0.0714
3	18.01	0.0170
4	22.65	0.0254
5	26.23	0.0144
6	28.66	0.0287
7	29.73	0.0243
8	30.81	0.0135
9	33.17	0.1088
10	36.74	0.0827
11	39.71	0.0769
12	42.11	0.0651
13	44.61	0.2639
14	47.95	0.1087
15	51.28	0.0988
16	52.8	0.2646
17	53.84	0.1835
18	56.05	0.3321
19	58.49	0.1968
20	58.68	0.1645
21	61.64	0.4736
22	63.94	0.1194
23	66.63	0.7212
24	72.17	0.3312
25	78.02	0.1548
26	83.08	0.0187
27	85.91	0.2491
28	94.16	0.9357
29	94.65	0.4326
30	96.7	0.1662
31	100.95	2.0765
32	120.21	0.9568
33	131.83	1.7638
34	135.7	1.7617
35	139.76	2.5333
36	245.26	2.2957



37	254.94	4.6358
38	266.22	6.6307
39	2120.56	884.0235

---

**CO\_Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.77	0.0160
2	14.6	0.0326
3	22.4	0.0902
4	23.01	0.0071
5	28.35	0.0157
6	29.72	0.0014
7	32.11	0.0086
8	33.59	0.0096
9	34.12	0.0163
10	35.94	0.0250
11	39.4	0.0272
12	40.67	0.0353
13	42.92	0.4044
14	45.27	0.0013
15	46.51	0.0100
16	47.95	0.1368
17	50.61	0.4355
18	53.47	0.4384
19	54.33	0.4777
20	54.92	0.2959
21	60.52	1.0934
22	61.58	0.0114
23	64.36	0.5128
24	65.52	0.0034
25	68.59	0.0843
26	71.81	0.1770
27	82.08	0.1187
28	86.5	0.2591
29	90.2	1.2778
30	94.71	0.9436
31	96.41	0.1963
32	97.45	0.4978
33	108.67	1.0453
34	114.63	0.1288
35	120.77	1.1573
36	122.96	3.6187
37	138.83	0.3876
38	144.53	0.0371
39	248.56	2.7420

40	261.11	6.0122
41	270.51	5.0931
42	2125.12	829.7579

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**CO\_Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.53	0.0452
2	16.47	0.0082
3	21.25	0.0496
4	21.52	0.1153
5	25.49	0.0315
6	27.97	0.1061
7	28.8	0.0908
8	31.25	0.2897
9	33.69	0.0336
10	35.16	0.1074
11	37.77	0.0316
12	39.69	0.1516
13	40.86	0.6244
14	42.35	0.0134
15	43.34	0.2568
16	43.66	0.0871
17	47.91	0.0666
18	48.73	0.2372
19	49.48	0.1091
20	50.65	0.0434
21	51.97	0.4695
22	52.81	0.2639
23	54.16	0.0094
24	58.66	0.4448
25	61.1	0.1745
26	64.51	0.1528
27	66	0.2346
28	70.84	0.3409
29	75.2	0.4325
30	76.08	0.0453
31	80.2	0.1305
32	85.66	0.1498
33	90.81	0.4647
34	92.86	0.0286
35	95.7	0.0283
36	105.74	0.2292
37	109.35	0.0151
38	115.21	1.2939
39	115.5	3.2761

40	127.6	0.2374
41	138.6	0.4997
42	197.87	6.4699
43	214.21	0.8334
44	250.6	8.4937
45	2116.97	1217.3838

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**CO Au<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.9	0.2094
2	18.46	0.1231
3	19.9	0.0423
4	23.8	0.0380
5	26.48	0.0985
6	29.33	0.0923
7	30.2	0.0247
8	31.12	0.0564
9	32.63	0.0812
10	34.4	0.0108
11	37.26	0.0199
12	38.14	0.0538
13	38.88	0.0497
14	39.64	0.0913
15	40.15	0.0363
16	44.29	0.4249
17	45.59	0.1796
18	46.95	0.5741
19	47.6	0.0137
20	50.27	0.2560
21	52.09	0.4192
22	54.05	0.4285
23	54.31	0.1656
24	55.1	0.0156
25	58.75	0.1024
26	63.14	0.3504
27	63.34	0.1319
28	65.29	0.1275
29	70.08	0.2232
30	72.29	0.0674
31	80.2	0.1224
32	82.64	0.4199
33	83.74	1.2227
34	87.23	0.3233
35	94.93	0.9511
36	97.23	0.7554

37	98.82	0.6882
38	102.1	1.7188
39	118.18	1.8566
40	125.05	4.8074
41	133.32	2.2397
42	134.58	0.9049
43	140.12	0.0235
44	153.12	1.0540
45	249.95	8.7497
46	256.56	6.8523
47	267.69	10.9378
48	2145.2	913.1297

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**CO\_Au<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.8	0.1912
2	18.83	0.0407
3	20.14	0.1413
4	22.1	0.1259
5	23.6	0.1128
6	24.42	0.2575
7	26.61	0.0275
8	29.21	0.3305
9	29.36	0.0669
10	31.28	0.0236
11	31.58	0.0211
12	32.73	1.0915
13	34.85	0.0997
14	39.26	0.0042
15	39.58	0.1933
16	43.5	0.0619
17	45.16	0.0122
18	47.05	0.0429
19	49.17	0.2376
20	52.49	0.0049
21	53.74	0.0095
22	55	0.1663
23	55.05	0.1800
24	56.45	0.0799
25	58.23	0.1128
26	59.39	0.1088
27	61.46	0.1927
28	62.14	0.6239
29	65.77	0.5740
30	65.83	0.5140

31	67.47	0.0610
32	73.56	0.0280
33	73.85	0.2543
34	79.53	0.0015
35	86.38	0.0209
36	88.94	0.2035
37	92.7	0.1279
38	93.9	0.1476
39	98.55	0.2308
40	102.02	0.1550
41	104.8	0.1523
42	107.7	0.1402
43	110.34	1.6826
44	112.08	0.5015
45	117.73	1.0163
46	122.3	0.8713
47	122.78	0.1374
48	195.02	1.2650
49	196.66	13.7960
50	235.03	1.9755
51	2103.01	1164.7960

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**CO\_Au<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.63	0.0801
2	17.65	0.3562
3	21.22	0.0466
4	22.21	0.0186
5	24.06	0.0561
6	24.56	0.3850
7	25.32	0.0677
8	26.42	0.1618
9	28.66	0.2123
10	29.57	0.3183
11	30.89	0.1680
12	32.86	0.3249
13	33.67	0.0225
14	34.28	0.0119
15	36.17	0.0090
16	40.19	0.0691
17	41.06	0.2029
18	41.9	0.1180
19	44.57	0.0526
20	46.34	0.1124
21	48.31	0.0889

22	51.06	0.0484
23	51.98	0.1040
24	52.56	0.0899
25	53.5	0.1936
26	55.81	0.0057
27	58.85	0.5396
28	60.95	0.2674
29	62.41	0.7088
30	63.01	0.2950
31	64.6	0.1458
32	65.87	0.2557
33	69.96	0.0526
34	73.56	0.0038
35	79.19	0.2168
36	81.93	0.2524
37	83.35	0.0066
38	87.7	0.0483
39	90.02	0.0399
40	91.37	0.1171
41	96.22	0.1024
42	99.23	0.0191
43	102.52	0.5047
44	106.99	1.1515
45	109.58	0.1680
46	112.27	0.0968
47	116.23	0.4420
48	120.16	1.2042
49	126.17	2.5160
50	127.66	1.1254
51	191.6	2.9208
52	203.44	2.0328
53	224.48	4.7754
54	2110.73	1019.6276

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**CO Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.82	0.0474
2	14.47	0.0531
3	28.24	0.0126
4	28.57	0.0043
5	28.98	0.0085
6	30.45	0.1390
7	32.59	0.3006
8	33.46	0.1928
9	33.75	0.0814

10	33.91	0.0211
11	39.92	0.0644
12	40.17	0.1082
13	40.68	0.0522
14	43.19	0.1114
15	43.64	0.1209
16	43.97	0.1154
17	44.5	0.0677
18	44.92	0.1863
19	46.55	0.0260
20	49.58	0.7569
21	49.64	0.7316
22	50.22	0.5733
23	51.88	0.1372
24	52.52	0.2290
25	53.07	0.0208
26	54.54	0.0246
27	55.93	0.0030
28	56.42	0.0008
29	58.93	0.1255
30	59.91	0.0106
31	60.35	0.0803
32	61.03	0.1452
33	63.52	0.0311
34	64.6	0.0612
35	66.01	0.0558
36	72.77	0.0055
37	77.44	0.0984
38	79.28	0.1333
39	83.04	0.1971
40	85.34	0.0548
41	86.13	0.1054
42	87.4	0.0121
43	89.67	0.2462
44	90.5	0.1855
45	94.69	0.1810
46	94.92	0.1215
47	99.39	0.6501
48	105	4.6902
49	105.66	5.2953
50	110.74	3.8454
51	124.71	1.4682
52	125.05	2.2961
53	126.55	2.9160
54	141.4	0.2257

55	142.02	0.1613
56	147.2	0.0788
57	2088.49	94.3009

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**CO\_Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.32	0.0794
2	17.14	0.0617
3	27.99	0.0018
4	28.39	0.0035
5	29.03	0.0056
6	31.95	0.2344
7	32.17	0.2622
8	32.32	0.3004
9	34.09	0.0055
10	34.36	0.0012
11	40.86	0.0362
12	41.59	0.0233
13	41.63	0.0160
14	41.87	0.0397
15	41.94	0.0311
16	44.95	0.0291
17	45.82	0.0268
18	46.26	0.0165
19	48.08	0.0350
20	50.39	1.0539
21	50.87	1.2088
22	51.05	1.1748
23	51.62	0.4225
24	51.92	0.0504
25	53.82	0.0160
26	55.38	0.0406
27	55.95	0.0081
28	56.78	0.0197
29	57.79	0.0136
30	58.46	0.0867
31	58.81	0.1197
32	60.4	0.1971
33	62	0.0473
34	62.19	0.0465
35	63.03	0.0782
36	63.85	0.0453
37	71.58	0.0575
38	72.19	0.0007
39	72.73	0.0010



40	74.02	0.0006
41	79.43	0.0021
42	86.63	0.2466
43	87.77	0.0019
44	88.1	0.0065
45	90.61	0.0726
46	90.93	0.0086
47	96.34	0.2755
48	96.41	0.0953
49	96.79	0.0810
50	98.2	1.6407
51	107.73	9.1098
52	108.03	8.7755
53	108.05	8.6628
54	138.38	0.0031
55	138.71	0.0128
56	143.79	0.1969
57	144.14	0.1700
58	144.27	0.1856
59	149.95	0.0005
60	2086.82	61.7203

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**CO<sub>2</sub> Au<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	38.68	0.3976
2	60.23	0.0319
3	611.27	71.9806
4	627.42	27.6374
5	1310.04	0.1633
6	2303.69	587.8527

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**CO<sub>2</sub> Au<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	24.16	0.0424
2	25.24	0.0000
3	75.82	2.8433
4	77.98	0.9124
5	153.38	0.0073
6	602.31	62.7768
7	625.74	25.1083
8	1310.61	0.1546
9	2298.68	347.3479

---

**CO<sub>2</sub> Au<sub>3</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.48	0.0049
2	11.51	0.0632

3	16.49	0.1720
4	23.13	0.3319
5	61.73	5.4143
6	72.25	1.0193
7	97.46	0.0224
8	128.35	0.4117
9	605.77	47.3889
10	627.01	23.8210
11	1311.37	0.0958
12	2296.15	148.1799

---

**CO<sub>2</sub> Au<sub>4</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.59	0.0295
2	29.12	0.1188
3	31.5	0.0005
4	40.14	0.0001
5	59.4	3.9428
6	62.17	0.0846
7	77.55	0.4733
8	82.15	0.0171
9	87.72	0.6174
10	127.19	9.7951
11	140.26	0.0009
12	607.91	62.4113
13	617.8	13.4582
14	1311.34	0.0044
15	2297.55	343.1530

---

**CO<sub>2</sub> Au<sub>5</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.35	0.0973
2	10.29	0.0001
3	20.51	0.0062
4	25.66	0.0009
5	29.56	0.0940
6	48.98	0.2042
7	56.45	0.4577
8	63.16	0.6807
9	77.95	0.1324
10	79.72	0.2460
11	86.3	0.1250
12	107.03	0.0265
13	119.35	0.5634
14	147.34	4.8190
15	610.01	61.6766

16	619.08	11.7622
17	1310.94	0.0115
18	2295.43	318.5027

---

**CO<sub>2</sub> Au<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.9	0.0153
2	19.71	0.0361
3	25.71	0.0052
4	29.45	0.0009
5	30.53	0.1356
6	33.74	0.1471
7	53.8	0.2017
8	55.71	0.0491
9	59.72	1.1491
10	71.55	0.6207
11	72.89	0.3233
12	76.48	0.1351
13	95.46	0.0068
14	103.99	0.0003
15	113.75	0.0021
16	155.64	9.1948
17	155.87	9.5087
18	604.83	65.2700
19	618.9	15.4679
20	1310.24	0.0711
21	2296.71	365.2426

---

**CO<sub>2</sub> Au<sub>7</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.12	0.0152
2	12.96	0.0282
3	17.55	0.0600
4	22.27	0.0712
5	26.71	0.0255
6	29.62	0.1017
7	34.85	0.0221
8	37.49	0.0736
9	45.2	0.0464
10	53.74	0.2820
11	61.89	0.8136
12	68.97	0.1506
13	72.76	0.1685
14	82.07	0.3088
15	92.5	0.1161
16	95.6	0.0841

17	96.94	0.0960
18	126.57	1.3944
19	143.37	6.9634
20	158.97	6.2357
21	604.56	61.5537
22	618.73	14.1690
23	1311.04	0.0398
24	2296.39	361.3683

---

**CO<sub>2</sub> Au<sub>8</sub>**

---

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.58	0.0101
2	22.23	0.0000
3	23.42	0.0948
4	24.95	0.1137
5	28.63	0.1131
6	29.88	0.3212
7	32.42	0.0000
8	35.98	0.0004
9	47.93	0.0004
10	52.5	0.1938
11	53.74	0.3327
12	59.8	0.1361
13	64.9	0.3243
14	68.37	0.1683
15	70.01	0.0000
16	82.73	0.0166
17	87.02	1.1599
18	87.63	0.9333
19	105.43	0.0005
20	118.34	0.0000
21	153.29	13.3203
22	153.99	13.0859
23	170.19	3.6365
24	602.71	16.3873
25	603.64	49.8636
26	1309.8	0.0295
27	2292.13	307.9298

---

**CO<sub>2</sub> Au<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.67	0.0013
2	14.92	0.0700
3	22.84	0.0398
4	23.82	0.0213
5	28.22	0.0722

6	30.04	0.1172
7	32.67	0.0001
8	34.28	0.0024
9	35	0.0110
10	42.01	0.0002
11	43.39	0.0308
12	46.55	0.0022
13	49.47	0.0065
14	62.54	0.0044
15	67.05	0.0002
16	68.9	0.0559
17	76.31	0.6962
18	81.38	0.0864
19	82.13	1.2160
20	92.01	0.2088
21	92.63	0.1087
22	107.36	0.0004
23	116.53	0.1555
24	143.28	6.9767
25	144.77	9.7337
26	159.79	1.8776
27	603.35	57.6148
28	616.74	11.1663
29	1309.79	0.0525
30	2291.79	243.1444

---

**CO<sub>2</sub>-Au<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.89	0.0000
2	11.8	0.0514
3	13.64	0.0037
4	19.25	0.0422
5	20.98	0.0002
6	24.05	0.0000
7	24.69	0.0374
8	28.96	0.0008
9	30.38	0.0485
10	42.23	0.0428
11	43.95	0.0000
12	44.55	0.0961
13	48.7	0.0007
14	58.77	0.0426
15	66.64	0.3256
16	67.48	1.3776
17	68.68	0.0011

18	72.91	0.0020
19	77.55	0.0000
20	84.67	0.4915
21	86.43	0.0391
22	87.94	0.0022
23	92.01	0.2639
24	98.65	0.0000
25	105.77	0.7757
26	116.67	2.8567
27	133.07	0.0002
28	133.59	3.5914
29	134.83	0.0016
30	604.77	58.1780
31	616.15	9.3829
32	1310.32	0.0145
33	2292.23	193.8510

---

**CO<sub>2</sub>\_Au<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8	0.0002
2	10.73	0.0079
3	11.51	0.0343
4	12.5	0.0065
5	16.91	0.0235
6	18.59	0.0254
7	21.52	0.0314
8	26.66	0.0351
9	28.01	0.0041
10	33.65	0.0132
11	36.53	0.0188
12	42.41	0.0667
13	45.1	0.0256
14	46.35	0.0558
15	48.96	0.0705
16	54	0.3520
17	59.72	0.0741
18	62.89	0.1325
19	71.89	0.0618
20	74.46	0.2764
21	77.39	0.8295
22	79.69	0.5397
23	83.14	0.0741
24	86.44	0.1916
25	88.19	0.3221
26	100.12	0.1385

27	106.45	0.0569
28	111.73	3.4663
29	119.34	0.4209
30	131.93	1.1019
31	134.85	0.6508
32	144.7	2.5484
33	597.99	58.4171
34	615.55	8.6267
35	1309.78	0.0345
36	2291.09	188.2442

---

**CO<sub>2</sub>-Au<sub>12</sub>**

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Mode	Frequency	Infrared
1	8.14	0.0018
2	13.01	0.0291
3	18.89	0.0179
4	20.88	0.0410
5	24.44	0.1084
6	25.13	0.0360
7	28.84	0.2617
8	29.59	0.1513
9	33.02	0.1265
10	39.42	0.0199
11	40.74	0.1921
12	42.72	0.0197
13	45.35	0.8606
14	47.31	0.4607
15	47.4	0.1583
16	50.91	0.2886
17	52.24	0.5556
18	56	0.0069
19	57.12	0.0015
20	62.32	0.3275
21	64.41	0.1464
22	67.76	1.3557
23	70.87	1.0427
24	74.29	1.0995
25	80.39	0.3852
26	82.44	0.1018
27	87.29	0.6366
28	89.23	0.0414
29	95.83	0.4475
30	98.4	0.5135
31	101.55	3.0430
32	131.65	0.6783

33	137.22	0.9665
34	141.82	6.0456
35	148.42	5.8324
36	585.66	84.5364
37	613.2	12.0691
38	1310.6	0.4122
39	2296.14	310.7934

---

**CO<sub>2</sub> Au<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.14	0.0255
2	18.02	0.0458
3	18.5	0.2371
4	23.59	0.0364
5	25.59	0.0631
6	26.66	0.0335
7	27.69	0.0308
8	29.61	0.0300
9	32.17	0.0138
10	38.37	0.0087
11	39.56	0.0101
12	41.36	0.2463
13	42.48	0.2778
14	43.77	0.7305
15	45.17	0.0727
16	48.76	0.2465
17	50.63	0.2927
18	53.28	0.0054
19	53.62	0.0231
20	54.17	0.0040
21	57.37	0.0159
22	60.86	0.7002
23	62.66	0.0666
24	64.94	1.1763
25	69.26	0.4773
26	71.81	0.8319
27	74.37	0.0941
28	79.89	0.6433
29	82.94	0.5823
30	85.6	0.0648
31	90.76	0.4727
32	94.13	0.0742
33	98.93	0.4965
34	99.92	3.0017
35	119.5	0.1278



36	128.64	0.5241
37	139.33	4.2327
38	145.31	4.5086
39	586.7	82.4407
40	611.57	12.7641
41	1310.73	0.2007
42	2294.93	268.8952

---

**CO<sub>2</sub> Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.99	0.0511
2	10.89	0.0174
3	15.77	0.0531
4	17.48	0.0241
5	22.86	0.0704
6	25.46	0.0049
7	29.36	0.0002
8	30.66	0.0219
9	34.13	0.0148
10	34.26	0.0381
11	35.54	0.1560
12	36.64	0.0013
13	43.63	0.0927
14	46.78	0.0104
15	47.06	0.0053
16	47.67	0.3751
17	48.67	0.4582
18	49.12	0.2846
19	50.49	0.0321
20	55.89	0.1940
21	58.9	0.0092
22	59.56	0.1887
23	60.87	1.2224
24	62.31	0.1203
25	66.2	0.0423
26	68.96	0.0410
27	71.26	0.2559
28	81.84	0.9476
29	82.78	1.4933
30	87.78	0.0797
31	91.47	0.5410
32	92.11	0.4872
33	94.11	0.2525
34	96.26	1.6078
35	100.92	0.0455

36	102.85	0.3518
37	114.6	0.0684
38	118.08	1.6769
39	122.76	2.2879
40	135.69	0.3373
41	141.36	0.0458
42	581.49	96.7008
43	611.28	11.3594
44	1309.78	0.6049
45	2294.15	241.0389

---

**CO<sub>2</sub> Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.22	0.0101
2	16.3	0.0565
3	19.91	0.0165
4	22.12	0.0177
5	24.48	0.1626
6	27.47	0.0022
7	28.63	0.0069
8	29.67	0.0009
9	34.95	0.0375
10	35.42	0.0857
11	36.99	0.0134
12	37.84	0.1220
13	43.24	0.0073
14	44.82	0.0380
15	46.49	0.0877
16	48.14	0.1806
17	48.16	0.0236
18	50.1	0.0004
19	53.44	0.3016
20	53.76	1.5950
21	56.79	0.0619
22	56.87	0.0006
23	59.16	0.2643
24	59.72	0.0482
25	60.86	0.0561
26	61.63	0.0369
27	63.28	0.1217
28	65.71	0.0938
29	66.25	0.0083
30	69.51	1.0361
31	74.79	0.8232
32	77.98	0.3038

33	82.3	0.3024
34	85.97	0.1590
35	89.53	0.0609
36	91.17	0.1475
37	93.86	0.0399
38	95.46	0.0166
39	98.26	0.3771
40	103.24	0.9491
41	108.31	1.5785
42	113.47	0.1108
43	119.47	0.2852
44	129.07	0.1467
45	589.37	91.2361
46	614.93	11.3975
47	1310.14	0.4494
48	2293.83	213.8202

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**CO<sub>2</sub>\_Au<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.75	0.0453
2	16.09	0.0159
3	19.47	0.0103
4	22.46	0.0118
5	23.35	0.0075
6	26.45	0.0192
7	27.13	0.0102
8	28.17	0.0072
9	29.98	0.0406
10	31.64	0.1328
11	35.42	0.0227
12	37.99	0.0410
13	39.98	0.0201
14	40.25	0.0172
15	41.16	0.2586
16	42.39	0.0372
17	44.37	0.0208
18	46.48	0.1823
19	47.24	0.0271
20	48.58	0.0974
21	51.4	0.5490
22	54.37	0.2143
23	55.62	0.0978
24	56.76	0.1429
25	58.35	0.4327
26	60.5	0.2586

27	61.81	0.2535
28	62.37	0.0024
29	65.44	0.3670
30	69.28	0.6807
31	71.54	0.0549
32	72.21	0.0947
33	78.74	0.1286
34	82.79	0.1725
35	86.19	0.9294
36	87.94	0.3490
37	91.76	0.1952
38	92.36	0.0504
39	95.35	1.0205
40	100.31	0.0491
41	102.21	0.4695
42	102.66	1.3833
43	109	0.3381
44	120.34	0.9277
45	124.57	3.3268
46	127.84	1.2929
47	143.16	0.0997
48	588.74	86.8642
49	608.97	9.2100
50	1310.29	0.2200
51	2294.46	245.2355

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**CO<sub>2</sub>-Au<sub>17</sub>**

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Mode	Frequency	Infrared
1	12.12	0.0262
2	14.65	0.0115
3	18.95	0.0311
4	20.69	0.0841
5	24.75	0.0091
6	26.61	0.0137
7	30.72	0.0507
8	31.19	0.0202
9	34.07	0.1224
10	34.18	0.1343
11	35.17	0.0119
12	37.37	0.1686
13	38.03	0.0916
14	39	0.0220
15	41.33	0.0106
16	44.14	0.0379
17	47.41	0.0791

18	50.07	0.2780
19	50.99	0.0543
20	51.66	0.0611
21	53.46	0.0107
22	53.92	0.0455
23	55.13	0.1121
24	58.09	0.9783
25	59.21	0.0845
26	59.45	0.2626
27	59.92	0.0771
28	60.27	0.0165
29	62.32	0.7064
30	64.15	0.0708
31	66.12	0.1003
32	68.43	0.8007
33	72.77	1.2282
34	80.89	0.5709
35	82.33	0.3324
36	85.54	0.0222
37	86.64	0.0416
38	87	0.1715
39	89.56	0.4135
40	90.44	0.0392
41	96.48	0.0340
42	98.77	0.3021
43	99.71	0.2371
44	102.77	0.1152
45	105.22	0.0857
46	105.7	0.2755
47	107.91	1.0808
48	112.49	0.8906
49	113.85	0.0152
50	120.82	0.0650
51	584.9	111.2353
52	609.22	12.0171
53	1310.61	0.4209
54	2294.88	260.9787

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**CO<sub>2</sub> Au<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.2	0.0819
2	19.92	0.2158
3	21.41	0.0112
4	24.59	0.0204
5	24.68	0.0189

6	27.05	0.0024
7	27.37	0.0921
8	29.09	0.2203
9	31.34	0.1977
10	31.99	0.0086
11	34.02	0.0503
12	34.09	0.0180
13	36.29	0.0079
14	36.97	0.2385
15	37.47	0.0038
16	40.4	0.0638
17	44.44	0.0042
18	44.58	0.0475
19	46.15	0.0663
20	46.79	0.1004
21	47.42	0.0872
22	50.91	0.1762
23	52.77	0.0047
24	54.01	0.4136
25	56.06	0.4916
26	56.68	0.4233
27	58.04	0.3391
28	58.44	0.0238
29	60.77	0.0465
30	62.38	0.0495
31	62.77	0.7023
32	64.44	0.1697
33	68.08	0.4490
34	69.27	0.1585
35	71.81	0.0785
36	74.19	0.4105
37	76.98	0.1045
38	82.26	0.1513
39	87.77	0.0057
40	89.57	0.0167
41	91.26	0.0184
42	94.59	0.0064
43	94.95	0.0413
44	96.3	0.0029
45	99.01	0.0322
46	101.04	0.0900
47	105.58	0.3768
48	107.75	0.1551
49	109.66	0.0059
50	111.77	0.2296

51	116.49	0.9538
52	118.52	0.4064
53	122.62	1.4148
54	584.49	114.0369
55	605.35	9.8081
56	1309.84	0.3650
57	2293.05	267.7678

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**CO<sub>2</sub> Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.13	0.0000
2	21.37	0.0060
3	28.88	0.0189
4	29.02	0.0004
5	30.5	0.0011
6	31.46	0.0786
7	32.58	0.2891
8	33.07	0.2915
9	33.52	0.0088
10	33.93	0.0071
11	39.67	0.0549
12	40.12	0.0640
13	41.55	0.0596
14	43.37	0.0711
15	43.44	0.0799
16	43.87	0.1589
17	44.53	0.3044
18	45.36	0.0541
19	46.88	0.0001
20	47.48	0.0270
21	49.79	0.6666
22	50.02	0.7007
23	50.21	0.3289
24	51.58	0.6346
25	52.54	0.0231
26	53.78	0.0024
27	54.9	0.0003
28	56.03	0.0026
29	56.81	0.0022
30	59.44	0.1065
31	59.95	0.0018
32	60.64	0.2301
33	62.2	0.0090
34	63.81	0.0012
35	64.68	0.0679

36	70.03	0.7100
37	73.33	0.0004
38	77.06	0.0262
39	79.03	0.5586
40	83.03	0.1819
41	85.68	0.0848
42	87.24	0.0015
43	87.4	0.2714
44	90.47	0.1141
45	90.53	0.0514
46	95.06	0.1533
47	95.35	0.2063
48	98.98	0.4307
49	105.54	5.1551
50	105.7	5.0112
51	124.54	1.7173
52	125.14	2.0275
53	125.6	3.1924
54	142.12	0.1489
55	142.47	0.1593
56	147.91	0.0795
57	590.86	75.7316
58	609.76	9.1063
59	1310.72	0.2076
60	2291.87	212.1991

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**CO<sub>2</sub>-Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.48	0.0003
2	22.07	0.0048
3	28.41	0.0013
4	29.37	0.0316
5	30.59	0.0414
6	31.49	0.1914
7	32.34	0.2237
8	33.5	0.2395
9	34.09	0.0117
10	34.43	0.0302
11	41.41	0.0307
12	41.47	0.0072
13	41.62	0.0035
14	41.85	0.0250
15	43.07	0.0225
16	45.78	0.0026
17	46.47	0.0044



18	46.74	0.0058
19	48.42	0.0024
20	49.39	0.0113
21	50.84	1.3393
22	51	1.2503
23	51.32	1.2146
24	52.09	0.0025
25	52.3	0.1062
26	53.38	0.0231
27	55.99	0.0014
28	56.58	0.0146
29	56.94	0.0187
30	58.4	0.0797
31	58.75	0.0764
32	58.98	0.0739
33	61.82	0.1023
34	62.11	0.0408
35	62.6	0.0379
36	68.79	0.3641
37	72.23	0.0005
38	72.93	0.0006
39	74	0.0011
40	75.32	0.3725
41	79.19	0.0459
42	81.73	0.5175
43	87.49	0.0015
44	88.54	0.0059
45	89.09	0.0789
46	90.92	0.0069
47	92.06	0.1848
48	96.47	0.1439
49	96.8	0.0170
50	97.04	0.0641
51	107.88	8.9630
52	107.94	8.8098
53	108.5	8.6973
54	138.37	0.0045
55	138.87	0.0014
56	143.66	0.1860
57	144.38	0.1715
58	144.55	0.1725
59	150.19	0.0023
60	594.98	81.9727
61	611.77	10.1360
62	1311.01	0.0679

63	2292.74	232.7801
<b>H<sub>2</sub>O Au<sub>1</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	39.71	386.0374
2	177.48	11.0588
3	318.3	41.9729
4	1572.34	102.1285
5	3757.7	0.3496
6	3937.28	106.5005
<b>H<sub>2</sub>O Au<sub>2</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	69.7	28.1617
2	69.73	10.3884
3	159.32	0.3570
4	177.4	379.2462
5	292.24	26.2174
6	483.92	42.1873
7	1600.34	132.9950
8	3789.2	17.5544
9	3952.56	152.7181
<b>H<sub>2</sub>O Au<sub>3</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.53	47.8428
2	36.23	6.7303
3	54.27	0.8587
4	66.92	4.4657
5	76.17	0.6371
6	144.49	1.2152
7	254.87	347.9570
8	299.92	19.4009
9	498.46	46.0785
10	1603.88	153.1526
11	3791.8	35.4850
12	3952.21	144.8246
<b>H<sub>2</sub>O Au<sub>4</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	27.68	0.2455
2	29.36	1.7270
3	54.29	2.7906
4	61.37	16.0649
5	64.7	2.4263
6	83.29	0.4532
7	90.54	0.0141
8	129.77	11.5065

9	139.76	0.1455
10	223.88	370.5187
11	299.09	14.8314
12	494.24	38.1310
13	1600.65	163.2858
14	3795.35	40.4199
15	3955.3	118.2663

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**H<sub>2</sub>O\_Au<sub>5</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.62	3.4731
2	21.44	0.0000
3	25.94	0.0780
4	38.46	20.1038
5	51.37	0.5899
6	51.56	0.2534
7	55.2	1.9494
8	78.45	0.0044
9	105.36	0.4353
10	111.1	0.0403
11	112.73	297.8465
12	121.03	0.3617
13	123.94	7.8427
14	226.54	2.8513
15	374.08	6.7369
16	1571	232.8139
17	3750.37	0.9419
18	3925.53	44.9780

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**H<sub>2</sub>O\_Au<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.7	0.1048
2	3.07	12.2943
3	28.8	0.0147
4	31.54	8.5821
5	32.42	0.0847
6	36.27	11.3627
7	47.43	1.0674
8	56.84	0.0656
9	63	0.7156
10	70.73	0.7894
11	93.05	135.0849
12	93.08	165.4633
13	101.6	0.0111
14	106.09	0.9055
15	144.95	9.3555

16	158.14	11.9176
17	200.13	8.7001
18	333.64	38.8590
19	1574.75	203.2397
20	3756.94	0.3893
21	3928.85	64.0361

---

**H<sub>2</sub>O Au<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.5	0.1594
2	19.39	0.1460
3	22.53	0.1043
4	26.64	0.2896
5	30.32	0.3671
6	43.35	3.6937
7	46.98	0.0857
8	54.02	0.3983
9	60.8	13.3409
10	67.74	0.4263
11	71.54	1.2191
12	85.41	0.9089
13	93.9	1.2763
14	98.13	0.5428
15	110.24	42.9149
16	124.35	31.1364
17	125.85	15.0917
18	141.6	11.0491
19	158.11	7.7064
20	304.36	5.4589
21	319.49	578.5865
22	1566.26	36.8440
23	3710.6	0.7515
24	3877.77	24.1312

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**H<sub>2</sub>O Au<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.03	0.0164
2	17.9	1.3107
3	24.53	0.0632
4	26.78	0.1597
5	29.41	0.0616
6	33.34	0.1701
7	51.47	0.1680
8	52.78	0.9538
9	59.19	0.2488
10	67.36	2.2443

11	70.23	0.2196
12	72.64	0.5467
13	76.82	4.0953
14	86.86	0.9542
15	87.66	1.0982
16	100.02	45.6142
17	105.89	1.5193
18	116.13	1.3621
19	148.11	4.1748
20	154.43	13.9126
21	169.1	5.8231
22	181.84	50.7488
23	295.86	166.3766
24	355.73	294.4900
25	1554.15	32.3658
26	3681.88	10.6480
27	3855.04	36.4172

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**H<sub>2</sub>O\_Au<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	1.02	0.0391
2	14.47	0.0082
3	21.71	0.0048
4	27.19	0.0042
5	28.88	0.0002
6	33.92	0.1536
7	38.38	0.5240
8	43.11	0.0801
9	49.55	0.0188
10	50.04	0.0056
11	57.07	0.7153
12	57.29	0.1614
13	69.36	0.0289
14	70.49	0.0926
15	77.19	0.7320
16	83.87	1.2456
17	87.67	3.3958
18	97.81	0.2155
19	102.18	0.9389
20	105.58	0.2391
21	131.62	2.4163
22	145.93	10.7288
23	159.72	9.7416
24	169.51	23.9819
25	183.04	39.0074

26	375.24	555.1053
27	433.7	9.1380
28	1583.58	49.3953
29	3709.73	2.3584
30	3868.57	33.6732

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**H<sub>2</sub>O\_Au<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.17	0.0146
2	13.61	0.0064
3	21.28	0.0112
4	24.46	0.3576
5	24.58	0.0007
6	27.37	0.3485
7	32.51	1.0948
8	39.29	0.0383
9	43.19	0.0453
10	45.01	0.0480
11	46.26	7.2958
12	47.86	1.0336
13	59.39	0.3279
14	65.46	1.0214
15	67.02	0.2364
16	68.62	1.3368
17	73.18	2.1913
18	76.4	0.0307
19	81.08	7.3148
20	85.03	0.0450
21	98.98	0.0009
22	104.51	8.9750
23	110.62	50.1802
24	116.88	3.6327
25	129.83	1.2810
26	132.32	16.0241
27	135.85	1.3051
28	168.86	39.6761
29	293.12	508.9818
30	309.74	0.9680
31	1570.62	20.9155
32	3709.61	0.8655
33	3874.96	14.9785

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**H<sub>2</sub>O\_Au<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.12	0.0202
2	10.6	0.0107

3	13.69	0.0623
4	20.99	0.0961
5	24.94	0.0654
6	25.51	0.0950
7	26.32	0.0274
8	34.95	0.0131
9	39.27	0.3833
10	40.62	0.3344
11	42.92	0.2568
12	47.49	0.0852
13	48.85	0.2370
14	54.04	0.2381
15	56.89	0.0474
16	61.66	0.1561
17	66.1	3.0699
18	71.55	0.8745
19	73.5	0.6918
20	80.36	0.3685
21	83.09	1.4285
22	87.77	0.5927
23	97.45	0.2401
24	101.85	0.8325
25	108.87	1.7244
26	111.38	1.7681
27	127.18	0.4067
28	134.71	1.2919
29	147.93	9.9943
30	151.76	25.5244
31	156.51	57.0454
32	333.36	557.6351
33	369.41	2.7116
34	1575.1	30.2999
35	3715.3	1.3144
36	3877.97	22.8235

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**H<sub>2</sub>O\_Au<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.09	0.0854
2	14.03	0.2018
3	18.61	0.0525
4	21.09	0.0605
5	27.1	0.1110
6	29.31	0.4742
7	31.06	0.1409
8	31.72	0.4505

9	34.02	0.0590
10	38.73	0.0923
11	41.93	0.2022
12	46.39	0.8663
13	50.43	2.6127
14	52.96	1.2026
15	54.31	0.3710
16	56.82	0.7865
17	63.61	0.4803
18	64.31	0.3234
19	67.13	1.0493
20	71.84	0.5173
21	78.93	0.1804
22	85.36	0.0458
23	90.19	0.2883
24	93.57	0.1056
25	98.71	0.2782
26	99.22	1.1906
27	109.36	4.0183
28	126.18	7.7089
29	136	6.4728
30	141.74	3.4203
31	148.34	15.7804
32	149.74	17.0298
33	153.83	110.6773
34	304.39	18.1192
35	424.64	69.3406
36	576.67	85.7139
37	1583	64.8205
38	3554.11	309.2641
39	3877.08	233.3286

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**H<sub>2</sub>O Au<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.18	0.7212
2	21.69	0.3740
3	24.48	0.0409
4	26.71	0.0349
5	27.46	0.0473
6	31.22	0.1731
7	34.03	0.0199
8	35.43	0.1469
9	39.83	0.0926
10	41.4	0.1256
11	42.92	0.6396



12	43.86	0.1251
13	44.44	0.0615
14	46.7	0.2943
15	50.56	0.5966
16	52.12	0.0722
17	52.18	0.0072
18	53.89	0.9579
19	58.86	0.1809
20	59.65	1.5673
21	62.4	0.4817
22	63.39	0.3884
23	67.04	0.9170
24	71.76	0.0907
25	74.66	0.3041
26	75.04	2.5957
27	83.15	0.0062
28	90.37	0.2694
29	91.04	0.9599
30	97.67	0.1317
31	98.77	2.5762
32	123.05	0.0467
33	132	1.3685
34	139.2	82.4189
35	140.04	67.4582
36	146.14	4.8163
37	226.31	10.4858
38	286.71	38.9362
39	465.87	142.4307
40	1562.43	220.1742
41	3673.62	52.9186
42	3870.28	105.5346

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**H<sub>2</sub>O Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.53	0.1583
2	17.91	0.0031
3	24.02	0.0411
4	29.49	0.3525
5	32.24	0.1862
6	32.3	0.1138
7	35.63	0.5475
8	36.91	0.0623
9	37.61	0.0644
10	38.21	1.8531
11	40.43	0.5666

12	42.09	0.9745
13	44.11	0.4446
14	48.31	0.3820
15	49.88	0.0158
16	52	0.3518
17	52.66	0.0169
18	53.65	0.0027
19	54.15	0.2672
20	58.4	0.0348
21	60.74	0.0370
22	62.47	0.2636
23	63.74	0.0227
24	65.95	0.5964
25	67.59	0.2777
26	82.25	0.2079
27	86.07	4.5649
28	88.03	0.6013
29	90.19	0.5498
30	95.29	10.1920
31	98.74	0.0321
32	100.52	0.1359
33	101.1	1.6349
34	117.4	8.6388
35	120.64	88.0739
36	126.99	2.0075
37	127.49	8.7365
38	137.18	0.3161
39	143.35	0.6076
40	277.28	13.8780
41	300.96	61.0685
42	505.82	127.8263
43	1579.07	208.9901
44	3691.41	67.1519
45	3893.68	246.4517

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**H<sub>2</sub>O\_Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.7	0.0297
2	19.16	0.2061
3	23.14	0.2393
4	24.35	0.1060
5	26.29	0.1301
6	26.9	0.0913
7	30.77	0.0498
8	33.27	0.0498

9	35.75	0.0758
10	37.96	0.0750
11	38.36	0.2548
12	42.32	1.2145
13	44.44	4.0488
14	45.3	0.8095
15	46.87	0.2077
16	47.81	0.1355
17	50.19	1.0526
18	51.15	1.1767
19	54.46	0.6417
20	55.36	0.2188
21	57.96	0.4226
22	60.13	0.0832
23	61.97	0.1564
24	62.12	0.3926
25	65.27	0.0581
26	67.74	0.2155
27	68.24	0.0344
28	76.81	2.9067
29	81.28	5.6327
30	82.75	3.0435
31	86.56	0.9143
32	90.41	0.5134
33	91.62	0.2425
34	92.97	0.8611
35	97.29	2.1191
36	99.03	11.6981
37	102.08	1.4635
38	103.11	61.4632
39	106.22	0.1350
40	117.27	3.2879
41	126.22	0.5193
42	142.26	0.1066
43	231.21	49.6935
44	262.2	19.4369
45	472.93	114.1939
46	1576.19	281.4642
47	3712.35	12.9169
48	3895.92	170.8279

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**H<sub>2</sub>O\_Au<sub>16</sub>**

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Mode	Frequency	Infrared
1	9.02	0.1790
2	16.94	0.4408

3	19.55	0.1052
4	21.52	0.1326
5	23.37	0.0530
6	26.85	0.7777
7	29.98	0.0068
8	30.62	0.0424
9	34.51	0.1561
10	34.95	0.0168
11	36.09	1.0468
12	38.21	0.0623
13	39.91	0.1973
14	42.32	3.7741
15	43.44	0.0821
16	46.26	0.0788
17	49.31	0.7358
18	49.79	1.8938
19	50.6	2.6426
20	53.56	0.3853
21	54.81	0.5959
22	56.03	1.2716
23	58.38	1.1164
24	60.62	0.3249
25	61.64	0.3248
26	64.53	0.1031
27	65.3	0.3637
28	68.43	0.0583
29	75.06	0.0701
30	78.12	0.6112
31	81.55	0.1873
32	84.26	0.2271
33	88.58	0.3892
34	91.76	7.2551
35	93.78	3.3448
36	97.7	1.6474
37	100.86	0.4074
38	104.32	2.5267
39	113.73	2.4832
40	118.91	13.2779
41	121.92	36.1783
42	125.22	65.5000
43	130.98	3.7048
44	138.76	0.5588
45	144.47	0.9664
46	259.51	29.6234
47	379.48	353.1881

48	535.16	100.3114
49	1596.52	49.9715
50	3666.24	54.2377
51	3870.54	155.9766

**H<sub>2</sub>O\_Au<sub>17</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.23	0.0940
2	17.79	0.9265
3	18.54	0.0645
4	23.35	5.8532
5	27.7	2.6016
6	28.22	0.1703
7	30.56	0.1019
8	33.43	0.5895
9	34.75	1.5423
10	35.22	0.2845
11	37.03	0.4951
12	38	0.4532
13	39.64	0.2766
14	42.12	0.4264
15	43.95	2.4042
16	47.1	0.3792
17	47.86	0.1649
18	50.38	0.2261
19	51.73	0.0336
20	53.02	0.0987
21	53.34	0.1676
22	54.66	0.2208
23	57.54	0.1067
24	59.06	0.1278
25	59.64	0.8232
26	60.47	0.1765
27	60.94	0.6795
28	62.42	0.1705
29	63.82	0.6283
30	67.23	0.0869
31	68.94	0.2192
32	80.3	0.6945
33	83	0.2870
34	84.65	0.1549
35	86.88	0.4134
36	87.54	0.2044
37	88.5	1.5766
38	92.21	2.4893

39	96.54	6.1706
40	97.52	12.4407
41	101.19	67.3588
42	104.51	0.0609
43	106.59	1.1148
44	107.18	0.6940
45	108.36	4.9042
46	113.11	1.1105
47	118.74	0.1448
48	122.74	0.1474
49	220.38	95.8697
50	253.39	150.2821
51	425.85	125.1402
52	1579.88	222.6110
53	3727.81	6.6279
54	3901.83	109.0692

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**H<sub>2</sub>O Au<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.51	0.8866
2	23.18	0.0353
3	24.63	0.2265
4	26.4	0.1343
5	28.49	0.2043
6	29.09	0.0695
7	29.89	1.1931
8	31.15	4.8538
9	32.22	0.1375
10	34.31	0.3783
11	36.46	1.4156
12	37.39	0.2243
13	39.07	0.0461
14	40.09	0.0803
15	40.98	0.1812
16	44.07	0.3790
17	46.18	0.5488
18	47.78	0.0463
19	48.59	0.0939
20	49.12	0.2546
21	51.12	0.1000
22	51.47	0.2403
23	52.82	0.0831
24	54.41	0.4963
25	56.91	0.5345
26	60.08	0.3553

27	61.8	0.1325
28	62.82	0.2680
29	63.3	0.7814
30	64.55	0.0203
31	66.42	0.1176
32	69.3	0.4674
33	74.13	0.2403
34	75.11	0.2989
35	80.6	0.0675
36	86.43	0.1275
37	88.63	0.0491
38	89.16	0.0938
39	91.58	0.5163
40	93.62	0.0061
41	95.31	0.0256
42	98.6	0.3047
43	99.12	0.0434
44	101.84	0.1937
45	106.89	0.8538
46	110.52	0.4519
47	115.26	1.6332
48	116.48	0.4078
49	121.71	0.0993
50	123.23	1.2610
51	128.48	119.9532
52	178.34	4.7731
53	253.93	97.8455
54	386.79	137.3804
55	1563.85	200.1345
56	3694.66	13.1066
57	3872.69	90.0535

---

**H<sub>2</sub>O Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.13	0.4708
2	25.8	0.0101
3	28.38	0.0588
4	28.5	0.3010
5	29.27	0.2632
6	30.08	0.0536
7	31.43	0.4465
8	33.34	0.0063
9	33.79	0.0748
10	37.36	1.1147
11	39.43	0.1101

12	39.74	0.0681
13	42.36	0.1098
14	42.92	0.1563
15	43.96	0.0747
16	44.19	0.9220
17	45.05	0.6717
18	47.29	0.7933
19	47.4	1.4466
20	49.16	0.6090
21	49.44	0.8899
22	50.8	3.2939
23	50.9	0.6130
24	51.85	0.0512
25	53.7	0.8839
26	55.06	0.0106
27	55.62	0.1232
28	57.05	0.7016
29	58.89	0.0062
30	59.66	0.0078
31	61.33	4.7435
32	61.65	1.1035
33	64.16	0.1691
34	65.4	0.2096
35	72.77	0.0518
36	77.02	0.0285
37	81.7	0.0324
38	84.02	0.1839
39	84.7	0.0320
40	87.11	0.0064
41	88.52	0.2215
42	91.38	0.3181
43	92.93	0.0886
44	94.58	0.2509
45	100.47	1.4310
46	104.01	1.4174
47	104.69	5.9954
48	108.15	30.0591
49	123.02	1.5265
50	124.96	1.9266
51	125.96	5.5877
52	139.7	19.9577
53	142.18	0.1294
54	143.64	77.8299
55	147.83	5.6334
56	291.98	629.4244



57	347.02	0.4563
58	1575.23	29.9338
59	3706.06	4.2689
60	3870.12	20.2213

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**H<sub>2</sub>O\_Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.84	0.6037
2	26.8	0.0483
3	28.74	0.0038
4	29.71	0.2014
5	30.1	0.1385
6	30.62	0.1473
7	32.18	0.1815
8	33.88	0.0460
9	35.31	0.2040
10	38.48	0.4827
11	40.84	0.0412
12	41.46	0.0067
13	41.75	0.0733
14	42.88	0.0529
15	45.77	0.2484
16	46.41	0.4045
17	46.95	1.5704
18	48.79	0.5124
19	49.69	0.5696
20	50.34	3.6877
21	50.59	1.4097
22	51.1	1.7500
23	51.94	0.1261
24	54.06	1.7919
25	55.03	0.0507
26	55.72	0.0265
27	56.69	0.0277
28	57.81	0.1335
29	57.99	0.2156
30	58.75	0.4086
31	59.5	0.2648
32	61.43	2.2052
33	62.22	1.2514
34	62.96	1.9558
35	71.7	0.0006
36	72.05	0.0210
37	72.64	0.0204
38	73.72	0.0043

39	78.76	0.1521
40	84.61	0.1197
41	87.69	0.0234
42	88.5	0.0105
43	89.7	0.1251
44	91.16	0.0812
45	95.87	0.0203
46	96.66	0.0467
47	97.19	0.0423
48	106.89	7.2825
49	107.21	9.3102
50	108.13	11.7269
51	126.63	35.4264
52	137.96	2.1275
53	139.25	0.2199
54	142.86	2.7145
55	144.12	2.1759
56	144.99	0.7225
57	147.08	70.6727
58	150.74	14.4894
59	301.8	643.5095
60	348.73	65.7260
61	1574.35	30.6266
62	3709.4	2.2788
63	3872.53	22.9887

---

**NO\_Au<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	268.15	1.4642
2	505.76	11.1582
3	1630.38	994.3710

---

**NO\_Au<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	2.97	26.7020
2	29.83	1.6497
3	133.16	2.7470
4	166.23	6.9810
5	221.42	12.7660
6	1856.72	548.7313

---

**NO\_Au<sub>3</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	47.47	1.3124
2	65.63	1.9116
3	77.53	2.6445
4	113.76	6.4662

5	135.18	1.1891
6	215.96	0.0769
7	274.93	6.7234
8	478.73	39.1710
9	1486.23	341.6275

**NO\_Au<sub>4</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.5	0.0562
2	26.32	0.0111
3	47.75	0.0010
4	60.07	2.5256
5	61.86	0.1981
6	82.38	0.0119
7	130.39	8.0336
8	136.26	0.7628
9	165.88	0.0565
10	173.13	0.5497
11	277.12	27.5717
12	1753.62	1807.6832

**NO\_Au<sub>5</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.08	0.2557
2	29.08	0.0649
3	39.32	0.4428
4	47.3	0.2332
5	50.9	0.3735
6	59.45	0.9803
7	74.25	1.1664
8	91.38	0.7844
9	98.9	0.9406
10	103.98	0.1254
11	128.04	3.7717
12	155.03	6.6565
13	259.8	0.8198
14	478.52	2.2261
15	1560.8	1773.0589

**NO\_Au<sub>6</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.45	0.1548
2	21.31	0.0296
3	23.59	0.0238
4	29.76	0.0527
5	30.91	0.0944
6	32.57	0.0637

7	54.05	0.1975
8	55.05	0.1998
9	69.02	0.2724
10	71.34	0.5737
11	72.06	0.7696
12	89.9	1.1281
13	95.92	0.0741
14	103.76	0.0201
15	113.64	0.0063
16	155.45	9.8476
17	156.09	9.2876
18	1844.66	87.2249

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**NO\_Au<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.24	0.2199
2	13.51	0.3578
3	17.61	0.2057
4	28.35	0.1192
5	32.93	0.4641
6	39.98	0.1703
7	45.49	0.2400
8	55.41	0.0765
9	55.82	0.2913
10	57.28	0.2198
11	68.09	1.0835
12	71.05	0.3710
13	79.44	1.5523
14	94.24	0.0297
15	104.65	0.4126
16	111.83	0.1075
17	151.4	7.5500
18	155.31	7.8314
19	268.07	0.3407
20	478.86	0.0502
21	1555.32	1505.8388

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**NO\_Au<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.84	0.0008
2	22.45	0.0077
3	23.27	0.0795
4	26.19	0.0625
5	27.24	0.2127
6	30.85	0.0792
7	33.07	0.0032

8	37.06	0.0235
9	47.16	0.1352
10	49.68	0.1303
11	56.26	0.1766
12	58.09	0.0755
13	62.74	0.2086
14	72	0.0004
15	78.41	0.0119
16	89.3	1.1820
17	89.52	1.1754
18	92.95	0.0120
19	107.71	0.0014
20	117.34	0.0035
21	153.71	14.8173
22	154.19	14.6855
23	170.75	1.3560
24	1861.66	48.2573

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**NO Au<sub>9</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.83	0.2317
2	19.95	0.1321
3	21.88	0.2077
4	24.5	0.2576
5	29.25	0.2163
6	36.99	0.1017
7	41.39	0.0335
8	47.09	0.3337
9	47.77	0.3460
10	52.71	0.7063
11	53.53	0.8761
12	58.31	0.1233
13	63.19	0.2329
14	68.93	0.6213
15	70.59	0.8957
16	81.7	0.3927
17	87.63	0.6638
18	105.52	0.2360
19	122.42	2.7557
20	139.45	1.2068
21	147.23	1.9043
22	157.39	5.4100
23	226.01	0.3148
24	247.41	11.0914
25	309.52	9.2879

26	500.21	0.6838
27	1481.23	230.6292

---

**NO Au<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	5.84	0.0965
2	11.1	0.0162
3	13.11	0.0189
4	18.47	0.0132
5	19.81	0.0054
6	21.62	0.0006
7	25.12	0.0199
8	29.15	0.0039
9	30.35	0.0366
10	38.71	0.0117
11	43.72	0.0008
12	44.75	0.0935
13	48.83	0.0012
14	58.67	0.0786
15	67.03	0.3234
16	67.26	1.1952
17	68.47	0.0033
18	72.22	0.1116
19	74.62	0.1358
20	77.39	0.0006
21	86.04	0.0207
22	87.16	0.0000
23	92.96	0.1670
24	98.81	0.0002
25	105.66	0.5506
26	116.26	3.0886
27	132.69	0.0011
28	133.29	3.6077
29	134.72	0.0431
30	1866.52	24.0332

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**NO Au<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.94	0.0130
2	11.34	0.0219
3	20.76	0.1121
4	24.33	0.1009
5	26.16	0.0161
6	30.53	0.0562
7	32.32	0.1344
8	36.83	0.3545

9	40.22	0.2479
10	44.47	0.0808
11	48.38	0.3879
12	51.89	0.2937
13	58.38	0.2136
14	61.07	0.3397
15	62.85	0.5975
16	68.31	0.3914
17	73.63	0.1783
18	80.08	0.6222
19	82.14	0.2550
20	85.56	0.9510
21	95.06	0.3750
22	96.49	0.3770
23	105.29	0.5418
24	110.1	0.7076
25	124.54	4.8072
26	142.57	5.3130
27	151.43	9.1811
28	157.9	8.4577
29	203.95	7.0775
30	215.6	1.0093
31	302.32	14.6281
32	483.25	0.2699
33	1462.64	290.2236

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**NO Au<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	2.53	0.0141
2	12.66	0.0050
3	18.6	0.0649
4	20.89	0.0202
5	22.65	0.0072
6	28.97	0.0509
7	30.25	0.0142
8	35.2	0.1603
9	36.11	0.6876
10	39.87	0.1287
11	40.9	0.0437
12	42.2	0.1302
13	46.1	0.2619
14	46.75	0.3394
15	50.3	0.1803
16	53.77	0.8554
17	53.9	0.0134

18	57.55	0.3456
19	60.17	0.2156
20	60.65	0.1449
21	65.1	0.1886
22	67.66	1.3532
23	71.75	0.1312
24	76.3	0.2417
25	84.5	0.0027
26	86.65	0.0412
27	90.26	0.0363
28	91.32	0.2849
29	96.27	0.4632
30	98.45	0.7572
31	101.28	3.2562
32	132.27	0.7133
33	137.43	0.9199
34	142.18	5.7486
35	148.52	6.1372
36	1863.68	56.0313

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**NO Au<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.05	0.0449
2	14.59	0.0320
3	17.79	0.0714
4	19.37	0.0540
5	24.87	0.0841
6	29.41	0.1813
7	31.47	0.2204
8	34.18	0.2304
9	37.57	0.0843
10	38.79	0.0932
11	44.2	0.1540
12	46.08	0.4134
13	47.51	0.5243
14	49.34	0.0850
15	50.9	0.1539
16	55.11	0.3118
17	55.96	0.3219
18	63.84	0.0904
19	65.41	0.3666
20	68.91	0.5907
21	70.12	0.2010
22	72.86	0.7131
23	77.06	0.6883



24	85.44	0.2820
25	87.04	0.7553
26	87.38	0.3030
27	93.24	0.2750
28	94.43	0.9077
29	110.14	0.0425
30	114.47	0.1263
31	122.04	9.3142
32	126.33	0.3198
33	139.35	1.6279
34	153.65	5.4580
35	184.32	4.2365
36	212.67	0.0787
37	285.81	15.6063
38	468.88	0.8714
39	1463.6	347.6325

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**NO Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.85	0.0122
2	15.58	0.0376
3	19.11	0.0095
4	20.66	0.0191
5	27.89	0.0872
6	28.89	0.0305
7	32.03	0.0762
8	33.38	0.0797
9	35.39	0.1267
10	36.22	0.1574
11	37.42	0.1045
12	40.56	0.1766
13	41.77	0.0695
14	43.25	0.0841
15	45.01	0.1455
16	46.63	0.3353
17	49.45	0.2730
18	50.97	0.4646
19	53.05	0.3201
20	55.05	0.2049
21	56.65	0.4534
22	58.86	0.3983
23	63.45	0.0735
24	65.53	0.0161
25	69.55	0.1264
26	71.35	0.1155

27	82.96	0.2276
28	87.74	0.4444
29	89.52	0.4771
30	94.84	0.1511
31	95.83	0.5412
32	99.18	0.7618
33	101.4	0.0254
34	102.08	0.4614
35	106.04	0.5218
36	113.62	0.0536
37	117.46	1.6460
38	120.96	2.8504
39	138.52	0.6921
40	141.65	0.0825
41	165.12	0.1890
42	1851.94	396.8672

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**NO Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.79	0.1042
2	14.99	0.2027
3	23.69	0.2144
4	25.98	0.0573
5	27.38	0.1292
6	27.9	0.2458
7	31.66	0.0340
8	34.14	0.1135
9	35.97	0.2055
10	36.89	0.0408
11	39.94	0.0158
12	41.04	0.1189
13	43.49	0.6556
14	45.84	0.0354
15	47.89	0.2054
16	51.45	0.0509
17	51.87	0.6579
18	54.19	0.2001
19	55.91	0.2823
20	59.37	0.1278
21	60.93	0.5687
22	62.91	0.3176
23	64.67	0.3064
24	65.75	0.3404
25	69.17	0.0957
26	71.29	0.1266

27	73.13	0.3536
28	76.82	0.2228
29	77.58	0.1536
30	85.43	1.0591
31	92	0.0199
32	94.49	0.2727
33	95.97	0.0150
34	97.94	0.2999
35	103.92	0.3997
36	108.57	0.5598
37	116.75	4.1866
38	119.53	1.4171
39	125.18	1.7731
40	143.96	0.0645
41	164.71	2.6513
42	195.83	0.4326
43	277.07	0.9741
44	484.03	0.6297
45	1496.45	522.8330

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**NO\_Au<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.71	30.6341
2	13.07	0.0447
3	16.46	0.0656
4	20.61	0.0278
5	21.44	0.0107
6	23.04	0.0233
7	24.4	0.0174
8	26.87	0.0125
9	27.29	0.0442
10	29.87	0.0113
11	32.18	0.2097
12	34.84	0.0547
13	38.48	0.0063
14	39.54	0.1647
15	40.41	0.0705
16	41.47	0.0705
17	44.48	0.0542
18	44.82	0.0208
19	48.4	0.1126
20	48.87	0.0241
21	51.48	0.2952
22	52.78	0.2348
23	54.57	0.4469

24	56.41	0.1514
25	56.97	0.1303
26	57.77	0.2355
27	60.51	0.2392
28	61.22	0.0342
29	65.3	0.1913
30	70.63	0.0388
31	70.89	0.0126
32	76.33	0.0972
33	79.5	0.3790
34	83.74	0.0373
35	88.66	0.3708
36	91	0.1143
37	92.77	0.3729
38	98.64	0.3837
39	99.26	0.1935
40	101.13	1.3784
41	103.74	0.2757
42	109.2	0.3696
43	117.67	1.3950
44	124.37	3.1504
45	130.3	0.7206
46	134.84	0.2943
47	142.21	0.2643
48	1415.76	46.4564

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**NO Au<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.38	0.1367
2	15.89	0.1413
3	17.99	0.0767
4	20.37	0.0689
5	24.36	0.1202
6	25.43	0.1958
7	29.09	0.1444
8	29.78	0.2178
9	32.81	0.0818
10	32.89	0.0934
11	34.1	0.7347
12	34.96	0.2023
13	35.29	0.1476
14	36.95	0.0119
15	38.42	0.0109
16	41.12	0.4192
17	46.01	0.2204

18	48.1	0.0628
19	49.84	0.2981
20	51.08	0.4107
21	51.59	0.0135
22	53.26	0.2427
23	53.59	0.0576
24	57.85	0.8041
25	61.26	0.0413
26	61.61	0.4296
27	64.03	0.0537
28	64.87	0.2053
29	67.29	0.2351
30	74.65	0.4174
31	75.49	0.0673
32	78.97	0.1076
33	79.88	0.2270
34	86.72	0.0986
35	87.37	0.0637
36	87.56	0.0296
37	94.75	0.1503
38	96.47	0.0397
39	98.79	0.0202
40	105.66	0.6962
41	113.38	0.1581
42	116.13	2.1807
43	120.78	0.3517
44	124.42	1.7747
45	125.35	2.6210
46	131.24	0.8609
47	163.22	5.4631
48	266.09	1.8074
49	267.79	11.1433
50	515.51	0.0876
51	1578.62	455.5611

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**NO Au<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.92	0.1047
2	14.32	0.0006
3	19.63	0.2276
4	21.68	0.0574
5	27.09	0.0080
6	27.64	0.1109
7	29.49	0.1743
8	30.52	0.0142

9	31.82	0.2511
10	33.5	0.0045
11	33.82	0.0187
12	36.28	0.0153
13	36.57	0.2107
14	36.9	0.0086
15	39.85	0.0566
16	42.35	0.2526
17	43.97	0.0144
18	45.05	0.0624
19	46.22	0.1984
20	46.75	0.1729
21	47.68	0.0618
22	50.84	0.1832
23	52.35	0.0227
24	53.66	0.0467
25	55.99	0.2075
26	57.94	0.0336
27	58.14	0.3759
28	59.15	0.0982
29	60.18	0.0884
30	62.53	0.3861
31	63.42	0.1418
32	64.26	0.2004
33	68.16	0.1481
34	69.37	0.1282
35	71.79	0.0987
36	76.29	0.0205
37	82	0.1629
38	87.77	0.0070
39	89.69	0.0179
40	91.04	0.0442
41	93.41	0.0211
42	95	0.0421
43	96.3	0.0061
44	98.6	0.0087
45	100.45	0.0193
46	105.02	0.2862
47	107.51	0.1993
48	109.09	0.0267
49	111.22	0.0957
50	116.52	0.9711
51	119.27	0.3161
52	121.96	0.9519
53	124.45	0.6549

54

1838.68

313.0351

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**NO Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.36	0.0107
2	23.58	0.1646
3	24.34	0.2306
4	27.68	0.0563
5	29.1	0.0588
6	29.89	0.0188
7	30.21	0.2504
8	31.22	0.0803
9	31.73	0.0867
10	33.72	0.0376
11	33.93	0.0483
12	36.26	0.4988
13	39.21	0.0132
14	39.37	0.0205
15	41.79	0.0554
16	42.6	0.0465
17	43.82	0.0035
18	45.4	0.0016
19	46.25	0.1064
20	47.54	0.3479
21	48.99	0.1728
22	49.5	0.5033
23	49.76	0.5830
24	50.01	0.3189
25	52.19	0.0013
26	53.14	0.0091
27	53.74	0.0102
28	54.39	0.0071
29	54.49	0.0064
30	57.99	0.0459
31	58.83	0.0821
32	58.89	0.0638
33	59.27	0.2293
34	66.12	0.1023
35	66.42	0.0960
36	72.26	0.0002
37	73.64	0.2261
38	81.72	0.0671
39	82.99	0.0718
40	83.16	0.1131
41	87.52	0.0036

42	89.34	0.2024
43	89.94	0.1646
44	94.56	0.0640
45	95.06	0.0525
46	98.35	0.0187
47	103.89	3.8188
48	104.25	3.5970
49	125.01	3.0665
50	125.55	2.9167
51	128.08	2.2051
52	132.23	7.3289
53	141.02	0.4863
54	141.16	0.4961
55	147.53	0.3313
56	276.06	2.8809
57	1540.76	3842.7221

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**NO Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	17.1	0.0642
2	23.09	0.0138
3	28.37	0.0007
4	28.9	0.0040
5	29.76	0.0898
6	31.54	0.2467
7	31.97	0.2373
8	32.21	0.1459
9	34.16	0.0078
10	34.34	0.0038
11	41.35	0.0118
12	41.53	0.0328
13	41.68	0.0238
14	41.77	0.0467
15	42.08	0.0404
16	45.76	0.0714
17	45.94	0.0017
18	46.62	0.0026
19	48.36	0.0245
20	50.59	1.1521
21	50.93	1.2459
22	51.2	0.9501
23	51.85	0.4119
24	52.08	0.0501
25	53.47	0.0596
26	55.8	0.1204



27	56.27	0.0385
28	56.52	0.0060
29	57.19	0.0907
30	58.59	0.1122
31	58.98	0.0575
32	59.23	0.2072
33	62.08	0.0465
34	62.11	0.0511
35	63.03	0.0454
36	68.01	0.2547
37	72.09	0.0011
38	72.53	0.0009
39	72.86	0.0009
40	73.96	0.0007
41	79.44	0.0069
42	87.2	0.0031
43	87.78	0.0122
44	88.39	0.0013
45	90.85	0.0065
46	91.13	0.0002
47	96.1	0.0437
48	96.58	0.0548
49	96.79	0.0741
50	106.9	6.0368
51	107.8	9.1353
52	108.01	9.2382
53	109.62	3.0763
54	138.3	0.0024
55	138.76	0.0059
56	143.61	0.1628
57	143.9	0.1683
58	144.53	0.1488
59	149.88	0.0011
60	1853.46	94.5049

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**NO<sub>2</sub>\_Au<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.46	2.8332
2	270.8	7.0519
3	373.5	9.2542
4	829.83	2.9449
5	1224.14	259.2925
6	1271.48	233.9566

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**NO<sub>2</sub>\_Au<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
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1	5.1	0.4240
2	61.34	0.0140
3	128.12	0.1544
4	186.24	0.0106
5	226.06	7.2705
6	254.41	6.6955
7	754.07	5.5554
8	1212.35	104.1980
9	1246.76	113.5483

**NO<sub>2</sub>\_Au<sub>3</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	41.27	2.4112
2	79.09	8.5590
3	90.31	1.0844
4	99.28	0.6996
5	102.88	1.7816
6	136.52	2.4182
7	216.32	18.6967
8	287.99	48.2871
9	335.45	3.0674
10	777.73	28.8283
11	1155.25	190.6157
12	1522.94	327.5341

**NO<sub>2</sub>\_Au<sub>4</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.59	0.2201
2	44.26	0.0989
3	50.63	1.8627
4	67.1	0.3896
5	82.95	0.6888
6	90.69	1.5708
7	116.56	1.2547
8	122.46	0.6404
9	153.44	4.2962
10	236.18	5.3036
11	300.21	48.1353
12	382.5	4.2749
13	791.43	27.8550
14	1176.59	179.2779
15	1522.88	314.3854

**NO<sub>2</sub>\_Au<sub>5</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.98	0.3963
2	31.84	0.0121

3	32.32	0.0846
4	44.69	0.2331
5	58.83	0.1582
6	69.46	0.2646
7	71.38	2.0312
8	91.44	0.6449
9	95.76	1.2573
10	109.65	3.3915
11	134.91	0.4702
12	151.89	5.6597
13	212.42	18.2680
14	242.01	13.3073
15	315.1	25.1651
16	826.67	19.9454
17	1000.58	741.9349
18	1528.11	294.2178

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**NO<sub>2</sub> Au<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.53	0.4775
2	13.15	0.0704
3	30.51	0.1175
4	31.26	0.0816
5	33.81	0.0472
6	41.82	0.1326
7	51.26	0.3913
8	62.55	0.3481
9	67.15	1.7440
10	88.33	0.3803
11	93.2	0.8226
12	93.29	0.8222
13	120.6	2.4651
14	123.77	0.0029
15	150.47	5.0244
16	215.01	34.0613
17	225.35	2.1002
18	334.46	18.5533
19	826.27	30.7413
20	996.57	897.0946
21	1531.58	346.3300

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**NO<sub>2</sub> Au<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.26	0.5021
2	23.81	0.0365
3	24.94	0.2786

4	31.82	0.2075
5	35.89	0.0012
6	38.32	0.0008
7	39.43	0.0941
8	54.14	0.2179
9	60.13	0.0351
10	74.6	0.1244
11	78.75	0.2485
12	92.68	1.1392
13	95.64	2.3634
14	109.22	0.2227
15	119.51	3.8415
16	131.57	0.4516
17	153.64	8.1166
18	163.94	7.0928
19	228.93	22.4089
20	232.6	1.4429
21	358.13	26.7660
22	831.95	39.5969
23	987.6	680.7322
24	1544.41	279.6716

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**NO<sub>2</sub>\_Au<sub>8</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.58	0.1123
2	17.6	0.5480
3	20.7	0.0197
4	26.93	0.0111
5	30.19	0.0680
6	33.59	0.0691
7	33.79	0.2334
8	40.73	0.0631
9	48.51	1.6279
10	55.61	0.6124
11	63.37	0.0493
12	76.66	0.0153
13	78.34	1.8093
14	79.86	3.3309
15	86.86	2.1645
16	94.24	2.5076
17	106.87	0.3055
18	113.86	0.7094
19	140.1	0.7178
20	144.64	5.0084
21	160.73	6.1004

22	221.34	24.2400
23	294.82	0.7831
24	315.83	27.7851
25	786.5	1.4439
26	1203.58	269.9924
27	1297.85	87.9574

**NO<sub>2</sub>\_Au<sub>9</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.13	0.1801
2	11.82	0.2403
3	18	0.0838
4	22.3	0.2816
5	24.39	0.0475
6	26.71	0.1644
7	28.4	0.0841
8	39.92	0.5526
9	46.11	0.3869
10	50.41	0.3166
11	53.96	0.0041
12	55.62	0.1961
13	62.28	0.1854
14	72	0.6934
15	73.07	0.3282
16	79.04	0.3752
17	91.95	0.9449
18	96.91	1.3266
19	115.07	2.8457
20	128.22	1.4792
21	131.65	0.2551
22	138.24	0.9080
23	159.79	3.5997
24	194.57	14.3061
25	242.66	4.3859
26	318.47	35.9838
27	381.18	4.7857
28	813.69	25.5830
29	1192.33	307.5308
30	1528	351.8125

**NO<sub>2</sub>\_Au<sub>10</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.46	0.0504
2	15.9	0.0413
3	19.63	0.2680
4	21.21	0.0506

5	28.27	0.0914
6	34.85	0.4252
7	36.6	0.4300
8	37.6	0.2994
9	44.08	0.0714
10	46.13	0.0369
11	49.51	0.5959
12	54.02	0.3896
13	56.51	0.4491
14	60.02	0.2333
15	63.43	0.1513
16	64.67	0.3016
17	73.1	0.0884
18	76.13	0.8752
19	81.81	0.9972
20	87.6	0.2770
21	94.49	0.6844
22	107.02	0.2087
23	115.45	0.2188
24	125.8	0.1348
25	134.72	0.9336
26	146.22	2.1624
27	194.27	8.3433
28	243.27	3.8161
29	297.51	25.0378
30	386.48	3.2903
31	818.15	22.2297
32	1214.35	178.6535
33	1508.89	318.8089

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**NO<sub>2</sub>\_Au<sub>11</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.65	0.0639
2	9.94	0.0670
3	16.57	0.1314
4	17.57	0.2431
5	18.66	0.0110
6	23.97	0.4248
7	26.39	0.0736
8	31.9	0.3800
9	37.04	0.4265
10	39.24	1.0771
11	44.09	0.5336
12	47.65	0.4249
13	55.02	0.7834

14	57.98	1.8205
15	58.5	0.3181
16	63.42	0.9097
17	68.32	0.7181
18	70.78	1.2153
19	75.43	1.1657
20	79.09	0.3258
21	82.35	0.1668
22	89.04	0.1871
23	94.91	3.7506
24	98.47	0.2148
25	100.46	0.0127
26	107.94	1.1863
27	118.27	2.1261
28	130.95	1.4027
29	138.67	3.5528
30	148.88	1.8342
31	158.06	4.0862
32	292.74	3.8079
33	336.48	13.9594
34	791.93	3.7522
35	1128.42	121.9592
36	1362.73	77.1071

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**NO<sub>2</sub> Au<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.77	0.6788
2	17	0.5274
3	22.65	0.1870
4	24.35	0.0439
5	26.41	0.1745
6	28.97	0.7528
7	30.99	0.6681
8	35.05	0.0747
9	35.59	0.1176
10	36.41	0.0785
11	39.8	0.2582
12	41.78	0.1802
13	43.17	0.1836
14	47.07	0.1122
15	48.25	0.0074
16	50.25	0.0139
17	54.25	0.5183
18	57.01	0.4953
19	60.23	0.9960

20	62.34	0.7465
21	68.34	0.6772
22	72.8	0.7284
23	74.3	0.3201
24	79.97	0.2866
25	84.55	0.7917
26	88.61	0.4341
27	93.74	0.5163
28	96.26	0.6096
29	105.75	1.3013
30	112.3	1.1137
31	135.1	1.2813
32	144.52	3.5952
33	148.84	7.1589
34	265.9	4.5338
35	279.55	43.4956
36	298.29	0.9429
37	775.57	0.1981
38	1250.54	212.8820
39	1273.16	3.7580

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**NO<sub>2</sub> Au<sub>13</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.45	0.0006
2	11.45	0.0263
3	18.19	0.0051
4	21.49	0.2806
5	23.89	0.1223
6	24.14	0.6307
7	30.05	0.0565
8	31.38	0.0043
9	32.94	0.0348
10	33.71	0.0217
11	39.12	0.3034
12	39.86	0.0143
13	40.79	0.0661
14	42.81	0.4248
15	44.15	0.4916
16	46.96	0.1210
17	52.96	0.1845
18	53.91	0.0219
19	57.8	0.1094
20	59.49	0.2725
21	65.18	0.1285
22	66.66	0.9181



23	71.17	0.1525
24	73.12	0.0283
25	86.74	0.3377
26	90.37	0.3233
27	93.5	1.9635
28	97.45	0.3231
29	103.17	2.1518
30	105.7	0.3615
31	113.8	0.4864
32	122.31	1.4385
33	139.68	1.5220
34	140.52	4.4901
35	148.89	8.9702
36	155.67	5.5170
37	216.39	7.3864
38	275.21	18.9063
39	327.9	9.1634
40	811.88	17.4293
41	987.42	379.6179
42	1521.54	166.3589

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**NO<sub>2</sub> Au<sub>14</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.2	0.0814
2	13.02	0.8608
3	15.32	0.7999
4	21.3	0.6956
5	24.82	0.0740
6	27.83	0.1722
7	32.62	0.0379
8	35.25	0.0123
9	36.06	0.1143
10	37.89	0.1624
11	39.39	0.1516
12	43.3	0.2037
13	44.6	0.1684
14	45.94	0.0269
15	47.07	0.2118
16	48.22	0.1262
17	50.87	0.0011
18	54.66	0.3051
19	55.29	0.3033
20	56.96	0.0273
21	58.12	0.2169
22	60.58	0.4462

23	61.19	0.0931
24	63.61	0.5603
25	67.04	0.0610
26	68.16	0.0736
27	70.22	0.3272
28	76.01	0.2359
29	83.48	1.0422
30	86.15	0.9506
31	92.05	0.2127
32	94.89	0.6064
33	98.27	0.4963
34	102.02	0.1197
35	105.74	0.6710
36	115.65	0.4058
37	123.54	0.7922
38	130.03	2.3982
39	138.77	0.5997
40	254.05	0.9044
41	276.19	50.9050
42	301.11	1.5229
43	780.2	0.5132
44	1244.04	140.7956
45	1272.23	12.1194

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**NO<sub>2</sub> Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	9.57	0.0302
2	19.2	0.0564
3	19.83	0.5974
4	22.43	0.0887
5	23.31	0.0020
6	29.67	0.0369
7	30.67	0.0161
8	32.69	0.0582
9	32.83	0.0059
10	35.91	0.0171
11	37.43	0.0384
12	39.13	0.9766
13	39.7	0.0554
14	40.15	0.1771
15	43.51	0.1952
16	44.88	0.3609
17	48.47	0.0000
18	49.29	0.2159
19	51.4	0.0020

20	52.91	0.1497
21	56.46	0.7038
22	57.87	0.3030
23	59.05	0.0724
24	60.82	0.1619
25	64.86	0.6085
26	67.98	0.2033
27	70.1	0.1202
28	74.06	0.0039
29	78.04	0.1200
30	83.71	0.0106
31	83.94	0.6554
32	91.32	0.0190
33	100.19	1.1633
34	100.28	0.1761
35	104.58	0.1392
36	117.37	1.0435
37	124.01	0.1031
38	129.57	1.2897
39	133.86	7.6704
40	135.78	1.2261
41	145.01	5.2185
42	176.29	4.8168
43	235.16	6.3565
44	306.03	62.0757
45	377.92	4.4537
46	800.71	39.3967
47	1211.98	222.4376
48	1512.86	472.6471

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**NO<sub>2</sub>\_Au<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.71	0.0150
2	20.34	0.1828
3	22.39	0.2300
4	24.73	0.0145
5	26.26	0.8595
6	27.53	0.3331
7	29.71	0.4462
8	30.52	0.0299
9	33.12	0.0655
10	35.69	0.1227
11	36.64	0.1590
12	38.11	0.0709
13	39.63	0.1388

14	41.37	0.1153
15	42.28	0.0813
16	43.89	0.0396
17	45.42	0.1084
18	47.18	0.1851
19	49.44	0.5996
20	50.05	0.2142
21	51.44	0.3225
22	55.09	0.2816
23	57.6	0.5261
24	58.36	0.4154
25	60.65	1.0329
26	64.74	0.2131
27	67.12	0.2980
28	68.73	0.1998
29	71.22	0.0781
30	75.07	0.6063
31	78.78	1.2990
32	82	0.4664
33	84.06	0.1148
34	85.66	0.6717
35	88.72	0.0111
36	89.26	0.1362
37	95.28	0.4385
38	103.02	0.4169
39	105.04	0.2557
40	113.56	1.7203
41	121.8	3.4543
42	129.26	1.5967
43	140.28	4.9104
44	140.76	1.1919
45	144.96	1.8540
46	226.88	10.9551
47	267.9	22.6788
48	308.86	7.9371
49	784.39	2.5162
50	1222.82	142.1520
51	1287.84	35.1917

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**NO<sub>2</sub> Au<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.86	0.0345
2	17.18	0.1319
3	19.34	0.0694
4	21.63	0.3320

5	24.22	0.0148
6	27.14	0.0545
7	30.89	0.0875
8	32.91	0.1724
9	34.28	0.3545
10	34.66	0.2714
11	38.26	0.1955
12	39.65	0.2569
13	40.32	0.0054
14	42.38	0.5824
15	43.58	0.1011
16	44.16	0.5446
17	45.73	0.0670
18	48.07	0.1486
19	50.8	0.0411
20	53.26	0.1051
21	55.23	0.1398
22	56.17	0.2560
23	58.29	0.2556
24	59.23	0.3249
25	60.86	0.7514
26	61.83	0.3054
27	65.33	0.9827
28	68.67	1.0465
29	69.51	1.0412
30	71.33	0.2377
31	74.86	0.4582
32	79.91	0.1873
33	81.14	0.1023
34	83.93	0.2169
35	85.89	0.0338
36	89.89	0.1959
37	92.35	1.4348
38	94.8	0.1686
39	99.92	0.9054
40	103.91	0.3407
41	109.91	0.9066
42	110.95	0.9851
43	117.07	5.4914
44	124.51	1.5324
45	132.29	5.9987
46	137.07	0.2792
47	143.7	3.3610
48	162.4	4.1976
49	219.92	10.6524

50	299.15	69.8495
51	339.78	6.0017
52	798.86	34.6594
53	1173.56	245.5612
54	1516.46	418.5790

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**NO<sub>2</sub>-Au<sub>18</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.75	0.1721
2	16.9	0.0815
3	19.09	0.0728
4	21.96	0.1014
5	23.89	0.0561
6	26.35	0.0553
7	28.63	0.0194
8	30.59	0.1198
9	32.53	0.0963
10	34.83	0.1487
11	35.77	0.0600
12	39.57	0.0727
13	40.46	0.1968
14	41.16	0.0151
15	43.34	0.1001
16	43.61	0.1719
17	44.5	0.0550
18	47.09	0.6104
19	47.9	1.5697
20	48.93	0.4484
21	50.52	0.0309
22	51.45	0.0421
23	52.56	0.0481
24	55.11	0.2358
25	57.49	1.3889
26	58.17	0.1190
27	59.49	0.3592
28	61.04	0.2805
29	63.93	0.0643
30	65	0.9211
31	67.07	0.0306
32	68.32	0.8343
33	74.45	1.4771
34	77.08	0.2265
35	80.31	0.2104
36	82.53	0.1710
37	86.08	0.2821

38	91.1	0.2680
39	92.86	0.0162
40	94	0.1317
41	95.4	0.0243
42	97.41	0.1412
43	99.71	0.3790
44	104.7	2.6203
45	114.5	1.2723
46	116.21	3.4202
47	127.14	1.1257
48	129.1	2.0840
49	132.11	0.2783
50	139.39	1.7669
51	142.62	0.8426
52	214.31	0.6647
53	240.32	34.2579
54	262.82	26.5366
55	769.75	2.9813
56	1150.09	254.6432
57	1326.12	85.6462

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**NO<sub>2</sub> Au<sub>19</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	20.22	0.0873
2	20.75	0.0943
3	22.48	0.2905
4	26.16	0.0715
5	26.45	0.3378
6	28.45	0.2516
7	29.88	0.1817
8	31.3	0.1831
9	32.34	0.2504
10	35.71	0.2191
11	36.35	0.0205
12	37.58	0.1002
13	40.37	0.3842
14	41.35	0.1903
15	42.88	0.6760
16	43.44	0.1390
17	44.31	0.4180
18	45.12	0.8417
19	46.16	0.1566
20	46.92	0.0735
21	47.32	0.4620
22	49.49	0.2943

23	50.96	0.3542
24	52.27	0.5586
25	53.23	0.1272
26	53.56	0.7497
27	55.08	0.0332
28	56.48	0.0706
29	57.84	0.0945
30	59.19	0.4105
31	62.4	0.0777
32	62.98	0.1199
33	65.8	0.3900
34	69.23	0.3608
35	69.68	2.0113
36	71.91	0.0299
37	72.62	0.1688
38	80.43	0.1751
39	83.34	0.3072
40	87.6	0.0840
41	89.62	0.1150
42	90.06	0.5234
43	93.66	0.0503
44	95.67	0.0165
45	100.73	0.0447
46	102.34	2.8389
47	102.72	1.0496
48	106.87	3.3039
49	131.42	2.7291
50	135	3.4947
51	136.69	5.0137
52	139.18	1.9580
53	141.56	2.0799
54	146.12	0.7478
55	202.47	16.9543
56	242.44	6.2242
57	257.28	21.8182
58	772.04	1.4276
59	1216.53	178.8238
60	1264.41	2.7435

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**NO<sub>2</sub> Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	18.11	0.8252
2	18.73	0.3039
3	23.98	0.4097
4	26.31	0.0302



5	26.34	0.1302
6	27.48	0.2705
7	29.07	0.1157
8	29.52	0.9658
9	31.43	0.1514
10	34.58	0.0953
11	37.65	0.0840
12	39.44	0.0474
13	41.55	0.0299
14	41.81	0.1363
15	44.87	0.9514
16	45.66	0.0061
17	46.83	1.0007
18	46.94	0.4362
19	48.35	0.2439
20	50.88	0.6464
21	51.3	0.1461
22	51.58	0.0726
23	51.86	0.2947
24	54.71	0.1962
25	55.18	0.0148
26	56.54	0.0575
27	56.8	0.2221
28	57.47	0.1064
29	59.44	0.0661
30	60.94	0.3043
31	61.06	0.0035
32	61.79	0.0490
33	64.7	0.0003
34	68.08	0.8170
35	70.19	0.2570
36	72.45	0.0193
37	74.49	0.0291
38	75.45	0.0535
39	77.08	0.1803
40	79.6	1.3363
41	88.29	0.2901
42	88.58	0.0054
43	90.98	0.1293
44	94.44	0.2317
45	95.86	0.1539
46	96.6	1.1220
47	102.2	3.2261
48	105.03	0.2980
49	106.8	1.5443

50	109.07	11.2035
51	117.5	5.5543
52	119.68	5.8396
53	138.18	0.0934
54	141.03	0.3058
55	143.41	0.0448
56	144.26	0.9035
57	148.75	0.0781
58	175.27	5.7667
59	235.65	65.1846
60	292.28	0.8842
61	753.62	31.8745
62	1096.83	243.3986
63	1530.21	339.2891

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**SO<sub>2</sub>\_Au<sub>1</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	8.23	2.6900
2	180.52	34.4730
3	249.77	10.6170
4	483.07	30.4130
5	790.03	173.2239
6	859.86	21.5139

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**SO<sub>2</sub>\_Au<sub>2</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	53.67	8.9805
2	75.53	2.9971
3	99.02	1.6492
4	215.55	13.6947
5	354.04	44.1554
6	357.53	18.5231
7	425.04	0.5116
8	726.22	285.5627
9	800.89	26.5325

---

**SO<sub>2</sub>\_Au<sub>3</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	37.75	0.6435
2	59.69	5.6515
3	91.77	0.2428
4	95.11	0.0002
5	99.88	0.1210
6	115.98	18.7379
7	143.33	1.6648
8	257.47	19.4979
9	314.85	3.9061

10	433.9	99.4392
11	844.8	137.0751
12	879.09	93.6458

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**SO<sub>2</sub>\_Au<sub>4</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	48.32	0.3054
2	49.83	1.6797
3	60.61	1.8358
4	67.54	0.3153
5	74.64	11.5242
6	76.66	0.3696
7	116.3	2.1649
8	131.63	7.3497
9	147.87	0.2879
10	284.98	17.0400
11	340.47	13.2136
12	365.44	4.4286
13	422.25	48.7174
14	709.49	58.1640
15	729.92	52.5275

---

**SO<sub>2</sub>\_Au<sub>5</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	16.02	0.0001
2	30.69	0.0982
3	37.86	0.0312
4	42.39	1.6621
5	58.05	0.7238
6	76.63	0.0073
7	76.84	0.0645
8	78.63	1.5764
9	92.22	0.1459
10	110.23	17.7442
11	111.49	0.5700
12	131.26	0.6302
13	162.26	8.6212
14	280.46	20.2377
15	325.77	0.2909
16	431.57	71.1274
17	887.27	181.2016
18	914.64	91.2761

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**SO<sub>2</sub>\_Au<sub>6</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	14.68	0.7255
2	18.47	0.1607

3	26.31	0.5279
4	26.96	0.3942
5	39.27	0.1187
6	42.88	1.0108
7	52.88	0.4922
8	56.45	0.4017
9	67.79	2.8783
10	68.58	0.4523
11	75.12	0.3281
12	90.87	0.5669
13	101.52	0.4836
14	110.37	0.5384
15	117.11	7.2012
16	150.79	6.8863
17	154.15	7.7547
18	171.78	43.1353
19	423.14	10.4546
20	929.38	58.5406
21	1043.11	67.3343

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**SO<sub>2</sub>\_Au<sub>7</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	13.29	0.4021
2	13.7	0.0055
3	24.42	0.9511
4	32.81	0.2082
5	38.4	0.0778
6	48.56	3.3838
7	50.2	2.3619
8	58.45	0.5686
9	62.07	0.0055
10	64.52	1.2472
11	65.48	0.4853
12	69.78	1.7842
13	80.02	0.5355
14	82.72	0.8566
15	88.66	0.3835
16	113.97	17.2533
17	119.37	0.3063
18	145.9	4.5130
19	154.61	5.7981
20	239.27	21.2835
21	322.3	1.4696
22	436.66	63.8096
23	854.22	114.9516

24

912.99

71.3107

**SO<sub>2</sub>\_Au<sub>8</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.3	0.0514
2	19.34	0.0105
3	19.56	0.2948
4	22.91	0.0154
5	23.07	0.0379
6	24.77	0.0487
7	36.25	0.7746
8	49.18	0.8334
9	50.88	0.3227
10	57.54	0.2787
11	59.55	0.3794
12	65.75	0.6002
13	71.63	0.9182
14	72.76	0.0018
15	85.51	1.4619
16	87.26	0.7746
17	98.76	0.8761
18	103.92	0.1418
19	109.58	0.3405
20	117.5	0.8979
21	148.82	10.9220
22	151.36	9.0702
23	165.18	15.9814
24	168.62	21.7219
25	422.94	20.1851
26	911.76	86.1421
27	1020.32	60.9126

**SO<sub>2</sub>\_Au<sub>9</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	6.55	0.0893
2	14.11	0.0497
3	18.16	0.0438
4	23.54	0.0457
5	31.12	0.1353
6	35.1	0.7058
7	40.25	0.2494
8	44.55	0.0751
9	46.62	0.4436
10	54.36	0.0078
11	59	0.1062
12	62.19	0.2858

13	66.55	0.4650
14	73.42	0.5902
15	74.73	0.8801
16	77.53	0.2689
17	83.68	1.8139
18	91.32	0.3361
19	98.68	0.4516
20	106.97	3.3533
21	109.75	9.3176
22	119.43	1.2968
23	141.74	11.9364
24	152.05	7.6990
25	163.67	3.3961
26	271.72	25.0185
27	321.98	1.7746
28	428.92	86.2212
29	869.59	143.0770
30	906.43	99.4783

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**SO<sub>2</sub> Au<sub>10</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.67	0.0017
2	16.87	0.0097
3	26.78	0.0616
4	29.7	0.0475
5	40.54	0.3183
6	41.23	0.3286
7	45.79	0.2702
8	46.28	0.0444
9	48.39	0.1654
10	49.07	0.4071
11	56.72	0.1229
12	58.19	0.2450
13	60.02	0.0804
14	63.02	0.2077
15	66.52	0.2079
16	74.91	2.4097
17	78.93	0.7533
18	85.5	1.3275
19	90.75	4.4373
20	99.15	7.3726
21	106.13	1.6092
22	128.2	1.8561
23	132.86	0.9835
24	136.36	3.0735

25	147.57	0.4398
26	170.29	6.4939
27	239.62	14.8760
28	283.19	10.4509
29	327.54	10.1114
30	373.87	30.4993
31	404.94	44.8292
32	691.97	63.0480
33	754.66	35.8118

**SO<sub>2</sub>\_Au<sub>11</sub>**

<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	11.54	0.0642
2	12.71	0.0537
3	16.22	0.1353
4	17.65	0.0263
5	24.38	0.4701
6	25.66	0.2474
7	29.36	0.1568
8	32.01	0.1356
9	36.26	0.1083
10	40.64	0.1038
11	43.31	0.3375
12	47.46	0.1812
13	48.66	0.1423
14	52.04	0.9636
15	57.22	0.2308
16	61.83	0.0653
17	68.58	0.2047
18	75.36	0.9373
19	76.27	0.0250
20	80.61	2.6903
21	84.87	0.6129
22	91.76	1.4901
23	98.08	0.1238
24	105.19	1.5796
25	120.23	7.4911
26	127.62	0.3170
27	136.42	0.8695
28	142.86	0.6944
29	148.99	3.8685
30	157.6	3.4762
31	242.45	10.8520
32	254.85	1.8915
33	357.6	32.0887

34	432.77	40.1561
35	801.56	114.3859
36	912.4	20.9272

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**SO<sub>2</sub> Au<sub>12</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	15.65	0.0478
2	19.81	0.1176
3	25.78	0.1314
4	30.84	0.0512
5	33.61	0.0143
6	37.6	0.2431
7	37.92	0.3012
8	39.09	0.4228
9	42.28	0.5722
10	45.14	0.0355
11	46.7	0.1246
12	48.9	0.4419
13	51.41	0.1057
14	54.97	0.5693
15	57.4	0.0083
16	58.18	0.2349
17	63.92	0.1636
18	68.5	0.3880
19	72.23	0.2585
20	79.44	0.2600
21	82.28	0.7271
22	85.28	0.6368
23	89.39	1.3365
24	91.12	0.1706
25	97.32	3.1428
26	111.1	0.7589
27	120.87	1.9427
28	131.77	2.8106
29	141.64	2.2386
30	145.87	3.8675
31	153.68	2.3178
32	171.37	3.6776
33	184.16	22.2629
34	232.5	12.3162
35	264.67	2.2893
36	369.35	75.9624
37	465.9	19.6128
38	657.03	63.9130
39	759.08	41.4709



<b>SO<sub>2</sub> Au<sub>13</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.75	0.1812
2	10.71	0.0317
3	13.11	0.0494
4	18.36	0.0838
5	19.38	0.0333
6	21.6	0.2095
7	24.98	0.0907
8	28.12	0.0198
9	29.43	0.0441
10	32.47	0.1773
11	35.17	0.1024
12	38.44	0.0537
13	39.56	0.1481
14	40.49	0.2182
15	47.01	0.3629
16	49.41	0.0801
17	53.27	0.1832
18	58.28	0.4086
19	58.45	0.5691
20	59.97	0.1484
21	64.49	2.5667
22	66.01	0.2006
23	68.35	1.7385
24	69.04	0.2073
25	77.23	0.0907
26	86.78	0.8110
27	92.26	0.4171
28	95.37	2.1149
29	97.71	0.5274
30	100.57	1.6171
31	107.1	0.8132
32	117.2	3.0907
33	121.96	2.7996
34	141.73	5.5088
35	142.94	0.5771
36	147.52	10.6383
37	158.61	5.2724
38	284.58	10.1849
39	319.06	6.9147
40	424.16	53.5730
41	865.17	111.8611
42	895.81	54.3956

<b>SO<sub>2</sub> Au<sub>14</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.78	0.0986
2	17.65	0.0628
3	21.33	0.1203
4	26.15	0.1103
5	29.27	0.1000
6	31.66	0.1159
7	32.32	0.0770
8	36.94	0.0855
9	40.02	0.1787
10	42.06	0.0286
11	43.8	0.6535
12	46.11	0.1881
13	49.68	0.8354
14	50.24	0.2984
15	52.52	0.0801
16	54.06	0.1951
17	57.73	0.0796
18	59.91	0.0374
19	61.66	0.0486
20	63.33	0.0993
21	63.92	0.2368
22	69.96	0.0822
23	71.5	0.5055
24	75.28	0.1807
25	77.32	0.4382
26	80.74	0.6043
27	88.32	1.3916
28	92.82	0.7384
29	97.18	1.6433
30	100.99	1.8209
31	104.35	0.4344
32	106.64	1.3722
33	116.15	1.4281
34	120.1	1.0061
35	127	5.7128
36	138.36	3.0095
37	149.67	2.5337
38	160.3	1.7611
39	196.34	9.9816
40	260.82	7.7702
41	311.67	21.3277
42	356.89	68.6386

43	399.25	11.3553
44	672.19	34.0978
45	742.07	15.7449

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**SO<sub>2</sub> Au<sub>15</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	12.02	0.0139
2	13.75	0.0187
3	18.47	0.0505
4	20.71	0.1088
5	25.21	0.0241
6	26.38	0.0189
7	28.83	0.1014
8	30.49	0.0326
9	35.02	0.2901
10	36.45	0.1301
11	37.81	0.2148
12	39.09	0.0837
13	41.3	0.0127
14	43.06	0.0719
15	45.79	0.0218
16	46.35	0.3486
17	47.48	0.0305
18	51.81	0.2570
19	52.44	0.0383
20	54.36	0.0850
21	55.52	0.3249
22	58.86	0.1601
23	63.47	0.0126
24	65.56	0.4693
25	67.37	0.1137
26	71.43	1.4388
27	73.87	0.1722
28	74.36	0.1409
29	77.09	0.4141
30	85.79	4.1155
31	89.91	0.1709
32	101.02	2.5907
33	106.61	0.1185
34	114.73	1.1756
35	121.26	0.2577
36	121.43	0.2120
37	131.71	1.0763
38	141.47	3.4432
39	146.34	0.2152

40	147.05	3.4170
41	176.76	1.8270
42	244.76	14.8539
43	263.08	7.5287
44	287.74	3.5943
45	372.59	42.0948
46	479.9	11.9885
47	689.88	50.5494
48	763.49	17.7720

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**SO<sub>2</sub>\_Au<sub>16</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	10.56	0.1296
2	14.18	0.1827
3	19.37	0.1129
4	21.17	0.0571
5	23.03	0.0361
6	24.29	0.0431
7	29.6	0.0365
8	30.84	0.0169
9	34.2	0.3839
10	35.52	0.1168
11	37.45	0.1358
12	39.14	0.1335
13	40.56	0.0705
14	44.51	0.2726
15	45.48	0.5400
16	48.31	0.4907
17	50.87	0.0895
18	51.53	0.0505
19	53.13	0.4716
20	56.48	0.0552
21	57.95	0.1829
22	61.06	0.0602
23	62.29	0.2489
24	64.88	0.0800
25	66.76	0.4427
26	68.34	0.1463
27	69.97	0.3548
28	72.46	0.3615
29	74.74	0.4770
30	80.79	0.3711
31	84.08	0.2748
32	87.31	0.3737
33	89.4	0.8423

34	96.69	1.4576
35	98.04	0.2543
36	107.04	4.5353
37	107.41	4.1237
38	114.33	1.5349
39	125.43	1.4814
40	126.79	1.0736
41	131.37	0.8070
42	138.95	1.3127
43	146.99	1.7573
44	161.98	2.7716
45	216.7	7.4637
46	261.22	3.3090
47	305.8	15.3886
48	358.77	43.4660
49	439.65	13.9803
50	692.93	51.2702
51	787.57	13.0861

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**SO<sub>2</sub> Au<sub>17</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	4.45	0.1110
2	8.29	0.3592
3	15	0.0514
4	21.03	0.1793
5	22.98	0.2748
6	26.3	0.0074
7	30.88	0.0293
8	31.6	0.0182
9	34.27	0.1066
10	36.25	0.1922
11	37.4	0.0319
12	38.89	0.0197
13	40.72	0.1456
14	42.39	0.0918
15	46.56	0.0056
16	50.65	0.0250
17	51.85	0.5317
18	52.3	0.0238
19	53.26	0.0785
20	55.91	0.5280
21	56.5	0.0968
22	58.74	0.1171
23	60.58	0.0698
24	60.92	0.1985

25	63.95	0.2641
26	65.75	0.1319
27	68.23	0.0915
28	68.66	0.6281
29	71.24	0.3414
30	71.56	0.3702
31	76.22	0.0906
32	78.27	0.0688
33	81.89	0.0625
34	82.59	0.2095
35	85.95	0.0885
36	88.69	0.2721
37	92.38	1.5177
38	95.37	0.2592
39	97.67	0.8217
40	101.09	1.4778
41	107.03	1.0092
42	110.32	1.2428
43	111.16	0.2155
44	114.28	1.2818
45	123.58	1.1096
46	136.09	2.6365
47	141.06	0.4608
48	144.79	0.2532
49	226.62	6.6436
50	230.13	29.2209
51	257.15	11.1160
52	419.43	63.5374
53	808.99	126.2992
54	898.6	20.1071

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**SO<sub>2</sub> Au<sub>18</sub>**

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Mode	Frequency	Infrared
1	4.81	0.7261
2	17.57	0.1660
3	18.85	0.8371
4	22.27	0.3168
5	23.2	0.0752
6	25.76	0.2468
7	27.47	0.4091
8	30.14	0.1431
9	30.42	0.1049
10	31.58	0.1955
11	34.17	0.0703
12	38.66	0.3174

13	40.43	0.2358
14	42.17	0.0262
15	45.02	0.0269
16	45.57	0.4103
17	46.38	0.3071
18	48.28	0.4631
19	49.76	0.2157
20	50.5	0.0350
21	51.65	0.8875
22	52.22	0.0333
23	52.74	0.3534
24	54.4	1.0073
25	56.6	0.1842
26	57.13	0.5183
27	58.27	0.4071
28	59.38	0.3234
29	61.51	1.6760
30	63.15	0.1893
31	64.39	0.2871
32	67.58	0.2361
33	72.77	0.2589
34	74.4	0.4152
35	77.16	0.0123
36	82.57	0.0006
37	85.33	0.2011
38	92.04	2.9007
39	93.28	0.7827
40	101.93	0.2551
41	103.28	1.6465
42	104.85	0.0640
43	108.38	2.8095
44	116.93	1.5917
45	118.63	0.7958
46	120.27	0.4272
47	123.12	0.1077
48	126.88	0.1276
49	140.28	0.4273
50	163.03	0.0065
51	177.37	3.5360
52	265.78	19.7160
53	316.4	26.7301
54	320.47	64.0384
55	393.18	11.5414
56	692.8	35.4773
57	731.49	18.3538

<b>SO<sub>2</sub> Au<sub>19</sub></b>		
<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	21.26	0.1053
2	22.59	0.0194
3	24.25	0.1274
4	24.39	0.1300
5	28.73	0.0595
6	30.31	0.0072
7	30.57	0.0878
8	30.8	0.0488
9	32.26	0.0178
10	34.37	0.1491
11	36.19	0.1442
12	36.32	0.0007
13	38.94	0.2738
14	41.08	0.0478
15	41.82	0.0651
16	43.98	0.1786
17	44.58	0.0765
18	44.86	0.6349
19	45.52	0.4139
20	47.76	0.5157
21	48.6	0.0374
22	48.89	0.1086
23	49.53	0.5818
24	51.45	0.1546
25	52.81	0.0934
26	53.14	0.3718
27	55.86	0.0050
28	56.32	0.0417
29	59.16	0.7522
30	59.68	0.4111
31	60.94	0.0915
32	61.93	0.0609
33	64.51	2.0212
34	69.85	0.0879
35	70.79	0.2518
36	72.85	0.4657
37	77.01	1.3145
38	80.78	0.1423
39	82.31	0.2044
40	85.19	0.0473
41	89.77	0.0548
42	90.33	0.5498



43	93.21	0.0046
44	95.24	0.0948
45	97.01	0.1594
46	99.16	0.8260
47	102.36	1.6213
48	103.21	3.5675
49	130.35	0.0001
50	134.19	2.7798
51	136.07	4.8871
52	139.18	3.6409
53	141.94	3.1967
54	145.1	1.6916
55	163.7	7.5212
56	193.19	24.1379
57	215.83	8.1147
58	416.7	64.1107
59	797.81	60.8153
60	881.35	25.2367

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**SO<sub>2</sub> Au<sub>20</sub>**

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<b>Mode</b>	<b>Frequency</b>	<b>Infrared</b>
1	7.91	2.3206
2	21.28	0.1258
3	25.77	0.0899
4	28.15	0.0495
5	29.8	0.9105
6	32.08	0.2386
7	32.51	0.1058
8	33.72	0.1340
9	34.73	0.1601
10	35.36	0.3803
11	37.9	1.1788
12	40.41	0.2461
13	40.74	1.6326
14	41.36	0.0927
15	42.77	0.1164
16	43.99	0.0143
17	45.11	0.3402
18	46.58	0.3208
19	47.58	0.5894
20	48.47	1.0835
21	49.01	0.5686
22	50.53	1.1966
23	51.03	0.2439
24	51.42	0.1799

25	52.91	0.4522
26	53.89	0.1169
27	55.39	0.1934
28	56.34	0.1098
29	57.1	0.0142
30	57.27	0.0906
31	58.12	0.1961
32	58.57	0.4041
33	61.42	0.0280
34	62.22	0.1788
35	64.3	0.2690
36	70.06	0.1315
37	71.66	0.1786
38	72.43	0.0731
39	73.63	0.1425
40	76.18	0.9871
41	79.23	0.0805
42	84.69	1.1760
43	86.73	0.1837
44	88.64	0.4221
45	89.24	1.1439
46	90.46	0.4438
47	94.98	1.3782
48	96.36	0.4989
49	97.6	0.6696
50	98.72	2.3184
51	106.66	7.7645
52	108.28	10.8581
53	109.54	8.3735
54	135.57	0.1707
55	137.51	2.7692
56	141.5	0.1248
57	143.66	0.8260
58	143.7	1.7650
59	148.94	3.1411
60	166.53	68.3637
61	420.08	4.8757
62	899.84	184.2525
63	1016.62	35.1580

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**Table S5**

Adsorption energies (kcal mol<sup>-1</sup>) of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, SO<sub>2</sub> with Ag<sub>n</sub> (n = 1-22) obtained from M06-2X/SDD level of theory

<b>Systems</b>	<b>CH<sub>4</sub></b>	<b>CO</b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub>O</b>	<b>NO</b>	<b>NO<sub>2</sub></b>	<b>SO<sub>2</sub></b>
<b>Ag<sub>1</sub></b>	-1.55	-4.48	-2.21	-8.12	-2.36	-55.23	-61.84
<b>Ag<sub>2</sub></b>	-2.93	-4.72	-5.67	-15.18	-5.31	-38.59	-18.96
<b>Ag<sub>3</sub></b>	-3.46	-12.98	-8.05	-18.85	-19.98	-78.52	-91.22
<b>Ag<sub>4</sub></b>	-1.63	-17.05	-8.41	-19.69	-11.86	-66.03	-84.08
<b>Ag<sub>5</sub></b>	-2.55	-7.83	-5.24	-13.07	-4.20	-76.74	-67.51
<b>Ag<sub>6</sub></b>	-2.54	-6.56	-5.19	-12.06	-6.95	-57.60	-83.66
<b>Ag<sub>7</sub></b>	-2.46	-9.04	-5.51	-14.41	-8.27	-61.73	-79.55
<b>Ag<sub>8</sub></b>	-2.83	-9.14	-5.59	-12.97	-5.30	-53.52	-83.04
<b>Ag<sub>9</sub></b>	-2.25	-9.69	-5.86	-12.09	-17.39	-55.66	-86.59
<b>Ag<sub>10</sub></b>	-3.69	-12.87	-6.99	-15.20	-26.26	-65.61	-96.58
<b>Ag<sub>11</sub></b>	-2.89	-5.84	-0.38	-14.11	-16.48	-63.99	-88.08
<b>Ag<sub>12</sub></b>	-3.43	-10.39	-7.57	-13.00	-14.54	-58.87	-96.79
<b>Ag<sub>13</sub></b>	-2.57	-4.80	-6.82	-14.33	-6.82	-65.76	-78.67
<b>Ag<sub>14</sub></b>	-2.73	-13.65	-6.73	-14.63	-9.52	-56.40	-92.44
<b>Ag<sub>15</sub></b>	-2.13	-5.05	-5.91	-13.76	-10.12	-65.87	-87.11
<b>Ag<sub>16</sub></b>	-2.82	-4.76	-6.89	-16.13	-23.56	-67.79	-97.98
<b>Ag<sub>17</sub></b>	-2.69	-4.98	-5.87	-16.58	-8.83	-68.40	-80.27
<b>Ag<sub>18</sub></b>	-2.59	-11.74	-6.49	-15.65	-7.04	-55.64	-90.52
<b>Ag<sub>19</sub></b>	-3.20	-5.00	-6.59	-14.52	-6.12	-61.84	-85.83
<b>Ag<sub>20</sub></b>	-3.16	-9.25	-7.15	-14.29	-7.57	-54.65	-85.74
<b>Ag<sub>21</sub></b>	-2.84	-5.12	-6.45	-13.46	-8.78	-68.98	-84.41
<b>Ag<sub>22</sub></b>	-3.26	-8.71	-7.19	-17.56	-9.50	-69.35	-90.87

**Table S6**

Adsorption energies (kcal mol<sup>-1</sup>) of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, SO<sub>2</sub> with Au<sub>n</sub> (n = 1-20) obtained from M06-2X/SDD level of theory

<b>Systems</b>	<b>CH<sub>4</sub></b>	<b>CO</b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub>O</b>	<b>NO</b>	<b>NO<sub>2</sub></b>	<b>SO<sub>2</sub></b>
<b>Au<sub>1</sub></b>	-1.71	-7.15	-2.32	-7.21	-6.30	-33.71	-37.67
<b>Au<sub>2</sub></b>	-4.84	-24.19	-4.42	-19.55	-10.19	-20.60	-26.12
<b>Au<sub>3</sub></b>	-3.65	-25.70	-4.86	-19.39	-9.37	-51.77	-72.58
<b>Au<sub>4</sub></b>	-5.66	-28.49	-6.59	-21.02	-15.77	-46.24	-52.73
<b>Au<sub>5</sub></b>	-2.95	-5.40	-5.31	-10.79	-7.46	-60.19	-80.99
<b>Au<sub>6</sub></b>	-3.21	-5.69	-5.65	-9.36	-6.07	-28.17	-13.31
<b>Au<sub>7</sub></b>	-3.47	-6.18	-5.99	-9.53	-9.24	-61.27	-65.41
<b>Au<sub>8</sub></b>	-3.80	-6.93	-6.87	-10.23	-6.86	-27.60	-15.33
<b>Au<sub>9</sub></b>	-3.93	-11.32	-6.66	-12.65	-8.94	-49.49	-73.96
<b>Au<sub>10</sub></b>	-3.68	-6.79	-6.50	-9.69	-6.78	-43.67	-76.92
<b>Au<sub>11</sub></b>	-3.68	-6.16	-6.64	-10.31	-19.35	-47.23	-69.12
<b>Au<sub>12</sub></b>	-4.01	-15.24	-6.22	-17.62	-6.54	-34.10	-62.49
<b>Au<sub>13</sub></b>	-3.25	-17.19	-6.27	-12.53	-6.90	-53.81	-64.49
<b>Au<sub>14</sub></b>	-3.29	-18.44	-6.40	-17.64	-7.70	-33.15	-59.69
<b>Au<sub>15</sub></b>	-3.49	-13.71	-6.35	-14.66	-2.37	-61.50	-70.21
<b>Au<sub>16</sub></b>	-3.59	-24.47	-7.43	-17.16	-7.39	-41.47	-68.64
<b>Au<sub>17</sub></b>	-3.04	-11.37	-6.11	-13.33	-4.52	-56.45	-64.52
<b>Au<sub>18</sub></b>	-3.15	-9.20	-6.18	-10.67	-6.42	-48.60	-61.64
<b>Au<sub>19</sub></b>	-3.57	-6.31	-7.15	-11.18	-12.88	-41.10	-53.14
<b>Au<sub>20</sub></b>	-3.62	-6.39	-7.21	-11.10	-7.13	-19.74	-16.72

**Table S7**

Interaction energies (kcal mol<sup>-1</sup>) of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, SO<sub>2</sub> with Ag<sub>n</sub> (n = 1-22) obtained from M06-2X/SDD level of theory

<b>Systems</b>	<b>CH<sub>4</sub></b>	<b>CO</b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub>O</b>	<b>NO</b>	<b>NO<sub>2</sub></b>	<b>SO<sub>2</sub></b>
<b>Ag<sub>1</sub></b>	-1.55	-4.51	-2.22	-8.15	-3.88	-73.10	-72.71
<b>Ag<sub>2</sub></b>	-2.99	-4.72	-5.71	-15.20	-5.41	-57.79	-29.42
<b>Ag<sub>3</sub></b>	-2.59	-14.49	-7.37	-18.49	-22.67	-95.11	-99.34
<b>Ag<sub>4</sub></b>	-1.64	-17.12	-8.51	-19.84	-18.58	-81.24	-144.27
<b>Ag<sub>5</sub></b>	-2.58	-7.93	-5.38	-13.58	-10.45	-92.01	-76.71
<b>Ag<sub>6</sub></b>	-2.60	-7.66	-5.42	-12.51	-7.00	-93.48	-141.53
<b>Ag<sub>7</sub></b>	-2.48	-9.46	-5.60	-14.70	-15.32	-75.89	-93.84
<b>Ag<sub>8</sub></b>	-2.90	-9.49	-5.70	-13.51	-5.42	-69.70	-130.41
<b>Ag<sub>9</sub></b>	-2.29	-10.17	-5.99	-12.69	-28.49	-76.90	-99.35
<b>Ag<sub>10</sub></b>	-3.76	-13.27	-7.13	-17.28	-22.93	-91.85	-144.80
<b>Ag<sub>11</sub></b>	-2.94	-5.94	-41.44	-14.70	-23.10	-82.13	-100.13
<b>Ag<sub>12</sub></b>	-3.48	-10.96	-7.83	-13.68	-36.38	-74.39	-148.23
<b>Ag<sub>13</sub></b>	-2.61	-4.84	-6.96	-14.85	-2.72	-80.20	-91.00
<b>Ag<sub>14</sub></b>	-2.78	-13.91	-6.80	-14.76	-9.88	-76.40	-151.44
<b>Ag<sub>15</sub></b>	-2.16	-5.09	-6.00	-14.22	-6.39	-83.87	-97.01
<b>Ag<sub>16</sub></b>	-2.87	-4.82	-7.10	-16.75	-34.33	-91.62	-136.05
<b>Ag<sub>17</sub></b>	-2.71	-5.05	-5.92	-17.03	-17.08	-89.74	-93.05
<b>Ag<sub>18</sub></b>	-2.60	-13.08	-6.57	-16.26	-7.11	-72.46	-129.23
<b>Ag<sub>19</sub></b>	-3.28	-5.07	-6.73	-14.74	-15.35	-81.87	-96.85
<b>Ag<sub>20</sub></b>	-3.20	-8.81	-6.60	-14.68	-7.67	-67.79	-130.55
<b>Ag<sub>21</sub></b>	-2.86	-5.17	-6.55	-14.36	-5.56	-87.70	-95.95
<b>Ag<sub>22</sub></b>	-3.34	-9.03	-7.36	-18.37	-18.77	-90.77	-134.21

**Table S8**

Interaction energies (kcal mol<sup>-1</sup>) of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, SO<sub>2</sub> with Au<sub>n</sub> (n = 1-20) obtained from M06-2X/SDD level of theory

<b>Systems</b>	<b>CH<sub>4</sub></b>	<b>CO</b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub>O</b>	<b>NO</b>	<b>NO<sub>2</sub></b>	<b>SO<sub>2</sub></b>
<b>Au<sub>1</sub></b>	-1.72	-7.20	-2.33	-7.25	-4.41	-50.02	-49.33
<b>Au<sub>2</sub></b>	-5.15	-24.37	-4.42	-19.69	-10.57	-34.36	-44.82
<b>Au<sub>3</sub></b>	-5.59	-28.96	-4.98	-21.86	-14.41	-66.65	-83.23
<b>Au<sub>4</sub></b>	-6.12	-29.22	-6.62	-21.70	-16.00	-62.06	-104.99
<b>Au<sub>5</sub></b>	-2.96	-5.44	-5.35	-11.78	-9.60	-88.70	-92.01
<b>Au<sub>6</sub></b>	-3.24	-5.72	-5.75	-9.87	-6.10	-70.35	-14.76
<b>Au<sub>7</sub></b>	-3.50	-6.26	-6.06	-10.43	-15.51	-98.59	-81.48
<b>Au<sub>8</sub></b>	-3.83	-6.95	-7.57	-11.24	-7.03	-47.40	-17.47
<b>Au<sub>9</sub></b>	-3.95	-19.89	-7.19	-15.72	-33.08	-87.76	-87.11
<b>Au<sub>10</sub></b>	-3.74	-6.99	-6.55	-9.54	-6.80	-97.41	-124.27
<b>Au<sub>11</sub></b>	-3.72	-6.25	-6.69	-12.27	-29.11	-75.88	-103.74
<b>Au<sub>12</sub></b>	-4.04	-21.64	-6.26	-25.31	-6.66	-56.61	-115.80
<b>Au<sub>13</sub></b>	-3.27	-22.09	-6.29	-15.24	-25.56	-94.04	-92.01
<b>Au<sub>14</sub></b>	-3.39	-22.67	-6.43	-21.47	-8.77	-55.16	-117.30
<b>Au<sub>15</sub></b>	-3.52	-17.42	-6.47	-19.48	-18.58	-78.92	-137.45
<b>Au<sub>16</sub></b>	-3.63	-21.68	-7.49	-21.70	-7.66	-75.20	-126.27
<b>Au<sub>17</sub></b>	-3.09	-15.73	-6.14	-25.75	-9.74	-83.70	-83.41
<b>Au<sub>18</sub></b>	-3.18	-15.44	-6.20	-12.26	-6.44	-83.34	-111.37
<b>Au<sub>19</sub></b>	-3.57	-6.36	-7.16	-11.53	-7.02	-62.08	-67.25
<b>Au<sub>20</sub></b>	-3.64	-6.41	-7.25	-11.50	-7.16	-43.56	-17.84

**Table S9**

Adsorption energies (kcal mol<sup>-1</sup>) of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, SO<sub>2</sub> with Ag<sub>n</sub> (n = 1-12) obtained from PNO-LCCSD/SDD level of theory

Systems	CH <sub>4</sub>	CO	CO <sub>2</sub>	H <sub>2</sub> O	NO	NO <sub>2</sub>	SO <sub>2</sub>
Ag <sub>1</sub>	-0.19	2.06	0.85	-2.41	1.24	-59.94	-16.65
Ag <sub>2</sub>	-2.68	-1.83	-3.46	-9.03	-0.16	-39.93	0.74
Ag <sub>3</sub>	-2.59	-3.30	-5.68	-12.84	-13.69	-81.70	-47.07
Ag <sub>4</sub>	-2.26	-15.86	-5.97	-12.36	-14.36	-61.72	-22.09
Ag <sub>5</sub>	-3.08	-5.65	-3.90	-5.51	3.45	-80.75	-31.35
Ag <sub>6</sub>	-3.52	-5.29	-4.59	-5.69	10.50	-55.15	-25.21
Ag <sub>7</sub>	-3.73	-8.65	-3.73	-8.77	-2.06	-66.93	-15.23
Ag <sub>8</sub>	-4.70	-8.52	-4.17	-6.84	6.99	-50.15	-26.85
Ag <sub>9</sub>	-4.53	-8.72	-4.30	-5.65	-0.75	-58.83	-18.36
Ag <sub>10</sub>	-5.79	-11.64	-4.14	-7.09	-0.45	-45.46	-29.66
Ag <sub>11</sub>	-5.98	0.76	-4.25	-7.49	-4.75	-65.79	-39.66
Ag <sub>12</sub>	-5.71	-10.97	-6.03	-6.02	-0.12	-56.52	-32.32

**Table S10**

Adsorption energies (kcal mol<sup>-1</sup>) of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, SO<sub>2</sub> with Au<sub>n</sub> (n = 1-12) obtained from PNO-LCCSD/SDD level of theory

Systems	CH <sub>4</sub>	CO	CO <sub>2</sub>	H <sub>2</sub> O	NO	NO <sub>2</sub>	SO <sub>2</sub>
Au <sub>1</sub>	1.40	2.66	1.20	1.62	-23.07	-43.24	-41.07
Au <sub>2</sub>	-9.96	-38.85	-2.70	-15.97	-5.70	-6.91	-51.01
Au <sub>3</sub>	-13.46	-44.40	0.11	-19.95	-24.89	-67.60	-21.09
Au <sub>4</sub>	-10.91	-41.65	-5.53	-16.43	-12.74	-23.37	-9.74
Au <sub>5</sub>	-6.39	5.00	-4.20	-5.03	-26.35	-65.69	-18.38
Au <sub>6</sub>	-7.65	-4.18	-5.85	-5.55	-10.63	-23.99	-2.42
Au <sub>7</sub>	-8.28	3.60	-5.93	-6.03	-18.04	-69.23	-20.36
Au <sub>8</sub>	-9.77	-5.93	-7.95	-8.27	-4.84	-25.26	-14.32
Au <sub>9</sub>	-9.94	-11.27	-6.72	-6.18	-10.14	-60.34	-24.38
Au <sub>10</sub>	-10.27	-6.54	-7.89	-6.89	-21.52	-12.95	-22.06
Au <sub>11</sub>	-9.77	2.24	-8.15	-5.57	-15.84	-47.90	-54.02
Au <sub>12</sub>	-8.37	-25.38	-6.32	-14.33	-5.30	-18.54	-43.49

**Table S11**

The values of zero point energy correction (ZPEC), thermal energy (in kCal/Mol), heat capacity,  $C_v$ , (in Cal/Mol-Kelvin), and entropy,  $S$ , (in Cal/Mol-Kelvin) for isolated  $Ag_n$  ( $n = 1-22$ ) and isolated  $CH_4$ ,  $CO$ ,  $CO_2$ ,  $H_2O$ ,  $NO$ ,  $NO_2$ ,  $SO_2$  as well as their complexes obtained from M06-2X/SDD level of theory

Name	ZPEC	Thermal Energy	$C_v$	$S$
Ag <sub>1</sub>	0.000000	0.889	2.981	41.294
Ag <sub>2</sub>	0.000352	2.101	6.866	62.017
Ag <sub>3</sub>	0.000715	3.607	11.752	87.33
Ag <sub>4</sub>	0.001198	5.397	17.672	97.242
Ag <sub>5</sub>	0.001662	7.194	23.567	116.245
Ag <sub>6</sub>	0.002236	9.006	29.416	128.75
Ag <sub>7</sub>	0.002793	10.791	35.349	136.923
Ag <sub>8</sub>	0.003256	12.588	41.246	151.642
Ag <sub>9</sub>	0.003669	14.38	47.158	170.793
Ag <sub>10</sub>	0.004097	16.186	53.027	187.941
Ag <sub>11</sub>	0.004649	17.978	58.938	197.684
Ag <sub>12</sub>	0.005166	19.78	64.819	210.929
Ag <sub>13</sub>	0.005675	21.578	70.711	223.733
Ag <sub>14</sub>	0.006181	23.385	76.576	237.805
Ag <sub>15</sub>	0.006642	25.174	82.499	251.549
Ag <sub>16</sub>	0.007108	26.972	88.391	265.477
Ag <sub>17</sub>	0.007698	28.781	94.247	278.799
Ag <sub>18</sub>	0.00809	30.57	100.173	294.209
Ag <sub>19</sub>	0.008771	32.383	106.017	303.249
Ag <sub>20</sub>	0.009485	34.192	111.873	309.973
Ag <sub>21</sub>	0.009664	35.964	117.85	328.783
Ag <sub>22</sub>	0.010136	37.775	123.701	344.598
CH <sub>4</sub>	0.045676	30.458	6.39	44.467
CH <sub>4</sub> _Ag <sub>1</sub>	0.046108	32.144	12.258	75.87
CH <sub>4</sub> _Ag <sub>2</sub>	0.046662	33.901	18.05	92.966
CH <sub>4</sub> _Ag <sub>3</sub>	0.046914	35.682	23.994	119.1
CH <sub>4</sub> _Ag <sub>4</sub>	0.047556	37.53	29.867	131.397
CH <sub>4</sub> _Ag <sub>5</sub>	0.048052	39.302	35.739	147.646
CH <sub>4</sub> _Ag <sub>6</sub>	0.048568	41.104	41.599	161.857
CH <sub>4</sub> _Ag <sub>7</sub>	0.048895	42.885	47.609	176.954
CH <sub>4</sub> _Ag <sub>8</sub>	0.049622	44.685	53.404	185.12
CH <sub>4</sub> _Ag <sub>9</sub>	0.049815	46.451	59.408	204.822
CH <sub>4</sub> _Ag <sub>10</sub>	0.050365	48.237	65.239	215.688
CH <sub>4</sub> _Ag <sub>11</sub>	0.051013	50.062	71.127	227.153
CH <sub>4</sub> _Ag <sub>12</sub>	0.051424	51.827	77.029	239.702



CH <sub>4</sub> _Ag <sub>13</sub>	0.051953	53.663	82.894	258.381
CH <sub>4</sub> _Ag <sub>14</sub>	0.052457	55.453	88.795	267.795
CH <sub>4</sub> _Ag <sub>15</sub>	0.052894	57.262	94.704	286.222
CH <sub>4</sub> _Ag <sub>16</sub>	0.053332	59.04	100.595	297.698
CH <sub>4</sub> _Ag <sub>17</sub>	0.05405	60.872	106.421	309.849
CH <sub>4</sub> _Ag <sub>18</sub>	0.05453	62.666	112.346	321.167
CH <sub>4</sub> _Ag <sub>19</sub>	0.055109	64.417	118.184	331.513
CH <sub>4</sub> _Ag <sub>20</sub>	0.055644	66.237	124.122	341.759
CH <sub>4</sub> _Ag <sub>21</sub>	0.055874	68.017	130.072	360.019
CH <sub>4</sub> _Ag <sub>22</sub>	0.056474	69.834	135.86	373.734
CO	0.004798	4.492	4.976	47.305
CO_Ag <sub>1</sub>	0.005201	5.869	9.777	71.296
CO_Ag <sub>2</sub>	0.005573	7.775	15.753	88.693
CO_Ag <sub>3</sub>	0.006378	9.33	21.384	103.598
CO_Ag <sub>4</sub>	0.007615	11.527	27.106	118.585
CO_Ag <sub>5</sub>	0.007454	13.253	33.316	141.335
CO_Ag <sub>6</sub>	0.007917	15.038	39.18	157.41
CO_Ag <sub>7</sub>	0.008618	16.853	45.066	166.449
CO_Ag <sub>8</sub>	0.009127	18.656	50.942	179.002
CO_Ag <sub>9</sub>	0.009556	20.454	56.86	194.015
CO_Ag <sub>10</sub>	0.010199	22.266	62.606	208.85
CO_Ag <sub>11</sub>	0.010113	23.897	68.753	222.139
CO_Ag <sub>12</sub>	0.01118	25.863	74.465	233.01
CO_Ag <sub>13</sub>	0.010963	27.551	80.585	255.863
CO_Ag <sub>14</sub>	0.012433	29.485	86.145	256.24
CO_Ag <sub>15</sub>	0.011973	31.153	92.381	279.987
CO_Ag <sub>16</sub>	0.012343	32.946	98.288	295.513
CO_Ag <sub>17</sub>	0.012976	34.76	104.14	308.556
CO_Ag <sub>18</sub>	0.014218	36.67	109.751	315.735
CO_Ag <sub>19</sub>	0.013993	38.359	115.921	332.279
CO_Ag <sub>20</sub>	0.015245	40.259	121.597	337.198
CO_Ag <sub>21</sub>	0.014866	41.939	127.76	359.693
CO_Ag <sub>22</sub>	0.015994	43.838	133.411	367.677
CO <sub>2</sub>	0.011174	8.676	7.02	51.234
CO <sub>2</sub> _Ag <sub>1</sub>	0.011313	10.138	11.993	79.424
CO <sub>2</sub> _Ag <sub>2</sub>	0.011972	11.972	17.842	93.964
CO <sub>2</sub> _Ag <sub>3</sub>	0.012396	13.774	23.749	118.138
CO <sub>2</sub> _Ag <sub>4</sub>	0.013027	15.579	29.607	130.009
CO <sub>2</sub> _Ag <sub>5</sub>	0.013135	17.252	35.659	146.251
CO <sub>2</sub> _Ag <sub>6</sub>	0.013631	19.059	41.515	160.856
CO <sub>2</sub> _Ag <sub>7</sub>	0.014156	20.817	47.503	171.675

CO <sub>2</sub> _Ag <sub>8</sub>	0.014834	22.741	53.229	188.282
CO <sub>2</sub> _Ag <sub>9</sub>	0.015041	24.42	59.285	204.204
CO <sub>2</sub> _Ag <sub>10</sub>	0.015631	26.254	65.109	217.821
CO <sub>2</sub> _Ag <sub>11</sub>	0.014749	26.925	71.287	224.776
CO <sub>2</sub> _Ag <sub>12</sub>	0.01668	29.795	76.968	237.112
CO <sub>2</sub> _Ag <sub>13</sub>	0.017133	31.612	82.846	253.049
CO <sub>2</sub> _Ag <sub>14</sub>	0.017489	33.378	88.775	268.516
CO <sub>2</sub> _Ag <sub>15</sub>	0.018277	35.324	94.474	285.797
CO <sub>2</sub> _Ag <sub>16</sub>	0.018486	37.015	100.523	296.773
CO <sub>2</sub> _Ag <sub>17</sub>	0.018988	38.789	106.43	310.65
CO <sub>2</sub> _Ag <sub>18</sub>	0.019469	40.596	112.313	323.671
CO <sub>2</sub> _Ag <sub>19</sub>	0.02009	42.383	118.209	332.17
CO <sub>2</sub> _Ag <sub>20</sub>	0.020854	44.257	123.958	350.269
CO <sub>2</sub> _Ag <sub>21</sub>	0.020985	45.982	130.009	360.157
CO <sub>2</sub> _Ag <sub>22</sub>	0.021449	47.733	135.951	371.823
H <sub>2</sub> O	0.021159	15.057	6.02	45.084
H <sub>2</sub> O_Ag <sub>1</sub>	0.022358	16.884	11.495	69.63
H <sub>2</sub> O_Ag <sub>2</sub>	0.02373	18.956	16.892	84.102
H <sub>2</sub> O_Ag <sub>3</sub>	0.024368	20.835	22.661	107.149
H <sub>2</sub> O_Ag <sub>4</sub>	0.025103	22.678	28.465	119.29
H <sub>2</sub> O_Ag <sub>5</sub>	0.024825	24.182	34.663	140.688
H <sub>2</sub> O_Ag <sub>6</sub>	0.025361	26.026	40.598	154.443
H <sub>2</sub> O_Ag <sub>7</sub>	0.026077	27.921	46.411	165.378
H <sub>2</sub> O_Ag <sub>8</sub>	0.026328	29.643	52.461	177.632
H <sub>2</sub> O_Ag <sub>9</sub>	0.02676	31.387	58.314	194.109
H <sub>2</sub> O_Ag <sub>10</sub>	0.027834	33.195	63.455	202.573
H <sub>2</sub> O_Ag <sub>11</sub>	0.02782	35.027	70.043	222.391
H <sub>2</sub> O_Ag <sub>12</sub>	0.028054	36.676	76.067	232.002
H <sub>2</sub> O_Ag <sub>13</sub>	0.028962	38.468	81.535	244.178
H <sub>2</sub> O_Ag <sub>14</sub>	0.029377	40.427	87.727	259.386
H <sub>2</sub> O_Ag <sub>15</sub>	0.029796	42.239	93.643	276.715
H <sub>2</sub> O_Ag <sub>16</sub>	0.030747	43.995	99.171	282.514
H <sub>2</sub> O_Ag <sub>17</sub>	0.031179	45.937	105.256	300.568
H <sub>2</sub> O_Ag <sub>18</sub>	0.031718	47.711	111.166	310.501
H <sub>2</sub> O_Ag <sub>19</sub>	0.031847	49.419	117.256	325.359
H <sub>2</sub> O_Ag <sub>20</sub>	0.032598	51.232	123.062	334.537
H <sub>2</sub> O_Ag <sub>21</sub>	0.032927	52.9	128.645	350.687
H <sub>2</sub> O_Ag <sub>22</sub>	0.033751	54.771	134.365	360.485
NO	0.004281	4.168	4.987	49.151
NO_Ag <sub>1</sub>	0.004975	5.434	9.318	67.214
NO_Ag <sub>2</sub>	0.005688	7.433	15.42	90.005

NO_Ag3	0.006456	9.118	20.892	100.504
NO_Ag4	0.007228	11.301	27.127	119.592
NO_Ag5	0.007295	12.62	32.694	131.876
NO_Ag6	0.007111	14.577	39.241	156.718
NO_Ag7	0.008499	16.296	44.397	156.981
NO_Ag8	0.008554	18.211	50.888	176.7
NO_Ag9	0.009609	19.929	56.106	185.767
NO_Ag10	0.008602	20.977	62.572	205.322
NO_Ag11	0.01049	23.483	67.942	212.801
NO_Ag12	0.009823	24.739	74.317	230.354
NO_Ag13	0.01039	26.567	80.192	239.661
NO_Ag14	0.011009	28.821	86.318	263.928
NO_Ag15	0.011381	30.17	91.934	270.004
NO_Ag16	0.012329	32.275	97.805	283.338
NO_Ag17	0.013355	34.241	103.31	294.783
NO_Ag18	0.01283	36.076	110.009	320.901
NO_Ag19	0.014468	37.86	115.078	318.338
NO_Ag20	0.014402	39.79	121.71	337.28
NO_Ag21	0.014371	40.972	127.273	347.162
NO_Ag22	0.015667	43.076	132.853	358.107
NO <sub>2</sub>	0.008114	6.95	7.006	57.58
NO <sub>2</sub> _Ag1	0.009365	8.603	12.118	71.935
NO <sub>2</sub> _Ag2	0.009549	10.358	18.13	95.671
NO <sub>2</sub> _Ag3	0.010504	12.198	23.944	103.805
NO <sub>2</sub> _Ag4	0.011025	14.039	29.78	121.911
NO <sub>2</sub> _Ag5	0.011609	15.886	35.588	137.421
NO <sub>2</sub> _Ag6	0.012151	17.675	41.477	149.26
NO <sub>2</sub> _Ag7	0.01286	19.63	47.445	161.639
NO <sub>2</sub> _Ag8	0.012825	21.187	53.439	178.7
NO <sub>2</sub> _Ag9	0.013327	23.019	59.517	191.79
NO <sub>2</sub> _Ag10	0.013806	24.789	65.217	207.082
NO <sub>2</sub> _Ag11	0.01438	26.639	71.296	218.073
NO <sub>2</sub> _Ag12	0.015307	28.62	76.922	231.654
NO <sub>2</sub> _Ag13	0.015803	30.41	82.822	243.889
NO <sub>2</sub> _Ag14	0.015513	31.816	89.058	257.76
NO <sub>2</sub> _Ag15	0.01685	34.019	94.59	270.9
NO <sub>2</sub> _Ag16	0.016579	35.423	100.79	284.149
NO <sub>2</sub> _Ag17	0.017239	37.332	106.501	299.726
NO <sub>2</sub> _Ag18	0.01816	39.404	112.291	315.473
NO <sub>2</sub> _Ag19	0.017946	40.828	118.494	324.56
NO <sub>2</sub> _Ag20	0.019496	43.036	123.999	334.876

NO <sub>2</sub> _Ag <sub>21</sub>	0.018902	44.399	130.313	350.482
NO <sub>2</sub> _Ag <sub>22</sub>	0.01962	46.24	136.092	363.022
SO <sub>2</sub>	0.005697	5.57	8.055	60.25
SO <sub>2</sub> _Ag <sub>1</sub>	0.006373	7.03	13.886	76.615
SO <sub>2</sub> _Ag <sub>2</sub>	0.006571	8.711	20.024	93.663
SO <sub>2</sub> _Ag <sub>3</sub>	0.007765	10.764	25.473	108.054
SO <sub>2</sub> _Ag <sub>4</sub>	0.008116	12.246	31.556	118.117
SO <sub>2</sub> _Ag <sub>5</sub>	0.008339	14.316	37.367	145.632
SO <sub>2</sub> _Ag <sub>6</sub>	0.00924	15.863	43.25	146.747
SO <sub>2</sub> _Ag <sub>7</sub>	0.009572	17.859	49.205	165.586
SO <sub>2</sub> _Ag <sub>8</sub>	0.010222	19.429	55.142	173.307
SO <sub>2</sub> _Ag <sub>9</sub>	0.010316	21.281	61.282	189.976
SO <sub>2</sub> _Ag <sub>10</sub>	0.011096	23.063	66.874	206.664
SO <sub>2</sub> _Ag <sub>11</sub>	0.011529	25.058	72.733	221.591
SO <sub>2</sub> _Ag <sub>12</sub>	0.012356	26.75	78.441	231.843
SO <sub>2</sub> _Ag <sub>13</sub>	0.012326	28.617	84.609	250.327
SO <sub>2</sub> _Ag <sub>14</sub>	0.013378	30.273	90.349	254.636
SO <sub>2</sub> _Ag <sub>15</sub>	0.01343	32.136	96.5	271.864
SO <sub>2</sub> _Ag <sub>16</sub>	0.014266	33.884	102.119	282.837
SO <sub>2</sub> _Ag <sub>17</sub>	0.014177	35.758	108.271	304.12
SO <sub>2</sub> _Ag <sub>18</sub>	0.015313	37.49	113.942	307.502
SO <sub>2</sub> _Ag <sub>19</sub>	0.015605	39.38	119.936	322.976
SO <sub>2</sub> _Ag <sub>20</sub>	0.016196	41.041	125.802	334.452
SO <sub>2</sub> _Ag <sub>21</sub>	0.016227	42.913	131.934	351.63
SO <sub>2</sub> _Ag <sub>22</sub>	0.017011	44.621	137.582	363.55

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**Table S12**

The values of zero point energy correction (ZPEC), thermal energy (in kCal/Mol), heat capacity,  $C_V$ , (in Cal/Mol-Kelvin), and entropy,  $S$ , (in Cal/Mol-Kelvin) for isolated  $Au_n$  ( $n = 1-20$ ) and isolated  $CH_4$ ,  $CO$ ,  $CO_2$ ,  $H_2O$ ,  $NO$ ,  $NO_2$ ,  $SO_2$  as well as their complexes obtained from M06-2X/SDD level of theory

<b>Name</b>	<b>ZPEC</b>	<b>Thermal Energy</b>	<b><math>C_V</math></b>	<b>S</b>
<b>Au<sub>1</sub></b>	0.000000	0.889	2.981	43.116
<b>Au<sub>2</sub></b>	0.000351	2.101	6.866	64.931
<b>Au<sub>3</sub></b>	0.000516	3.878	12.827	92.521
<b>Au<sub>4</sub></b>	0.001134	5.39	17.692	101.426
<b>Au<sub>5</sub></b>	0.001584	7.187	23.589	120.56
<b>Au<sub>6</sub></b>	0.002208	9.002	29.428	132.774
<b>Au<sub>7</sub></b>	0.00244	10.786	35.366	155.84
<b>Au<sub>8</sub></b>	0.003097	12.606	41.188	168.712
<b>Au<sub>9</sub></b>	0.003295	14.379	47.165	187.051
<b>Au<sub>10</sub></b>	0.003682	16.16	53.113	199.339
<b>Au<sub>11</sub></b>	0.004077	17.957	59.009	217.702
<b>Au<sub>12</sub></b>	0.004534	19.751	64.916	227.82
<b>Au<sub>13</sub></b>	0.004846	21.529	70.875	242.847
<b>Au<sub>14</sub></b>	0.005395	23.333	76.748	255.678
<b>Au<sub>15</sub></b>	0.00568	25.103	82.733	268.274
<b>Au<sub>16</sub></b>	0.006147	26.911	88.594	284.7
<b>Au<sub>17</sub></b>	0.006673	28.699	94.52	296.211
<b>Au<sub>18</sub></b>	0.007121	30.497	100.413	309.073
<b>Au<sub>19</sub></b>	0.007885	32.325	106.21	320.352
<b>Au<sub>20</sub></b>	0.00861	34.145	112.03	326.819
<b>CH<sub>4</sub></b>	0.04571	30.479	6.391	44.464
<b>CH<sub>4</sub>_Au<sub>1</sub></b>	0.046316	32.178	12.189	75.956
<b>CH<sub>4</sub>_Au<sub>2</sub></b>	0.046493	33.774	18.016	95.465
<b>CH<sub>4</sub>_Au<sub>3</sub></b>	0.046794	34.956	21.936	111.955
<b>CH<sub>4</sub>_Au<sub>4</sub></b>	0.047679	37.404	29.647	129.743
<b>CH<sub>4</sub>_Au<sub>5</sub></b>	0.04792	39.271	35.815	148.971
<b>CH<sub>4</sub>_Au<sub>6</sub></b>	0.048801	41.131	41.566	159.045
<b>CH<sub>4</sub>_Au<sub>7</sub></b>	0.049012	42.894	47.509	180.68
<b>CH<sub>4</sub>_Au<sub>8</sub></b>	0.049389	44.641	53.411	195.197
<b>CH<sub>4</sub>_Au<sub>9</sub></b>	0.049769	46.449	59.311	212.799
<b>CH<sub>4</sub>_Au<sub>10</sub></b>	0.050086	47.64	63.261	219.907
<b>CH<sub>4</sub>_Au<sub>11</sub></b>	0.050483	50.028	71.162	245.818
<b>CH<sub>4</sub>_Au<sub>12</sub></b>	0.050862	51.76	77.112	252.545
<b>CH<sub>4</sub>_Au<sub>13</sub></b>	0.051235	53.592	83.048	269.953

<b>CH<sub>4</sub>_Au<sub>14</sub></b>	0.051775	55.4	88.899	284.352
<b>CH<sub>4</sub>_Au<sub>15</sub></b>	0.052007	57.159	94.924	297.51
<b>CH<sub>4</sub>_Au<sub>16</sub></b>	0.0525	58.969	100.767	313.194
<b>CH<sub>4</sub>_Au<sub>17</sub></b>	0.053006	60.756	106.686	325.317
<b>CH<sub>4</sub>_Au<sub>18</sub></b>	0.053357	62.533	112.596	343.843
<b>CH<sub>4</sub>_Au<sub>19</sub></b>	0.054163	63.792	116.383	346.44
<b>CH<sub>4</sub>_Au<sub>20</sub></b>	0.055036	66.194	124.176	356.065
<b>CO</b>	0.004798	4.492	4.976	47.305
<b>CO_Au<sub>1</sub></b>	0.005487	5.914	9.618	70.701
<b>CO_Au<sub>2</sub></b>	0.007373	8.123	14.874	67.359
<b>CO_Au<sub>3</sub></b>	0.007718	9.884	20.742	106.323
<b>CO_Au<sub>4</sub></b>	0.008312	11.713	26.589	119.45
<b>CO_Au<sub>5</sub></b>	0.006994	13.165	33.447	147.558
<b>CO_Au<sub>6</sub></b>	0.00755	14.978	39.301	161.031
<b>CO_Au<sub>7</sub></b>	0.007719	16.762	45.255	184.892
<b>CO_Au<sub>8</sub></b>	0.008504	18.594	51.049	195.928
<b>CO_Au<sub>9</sub></b>	0.009788	20.555	56.461	208.718
<b>CO_Au<sub>10</sub></b>	0.009132	22.15	62.958	225.823
<b>CO_Au<sub>11</sub></b>	0.009344	23.928	68.895	246.655
<b>CO_Au<sub>12</sub></b>	0.011349	26	74.109	246.438
<b>CO_Au<sub>13</sub></b>	0.011536	27.747	80.104	262.839
<b>CO_Au<sub>14</sub></b>	0.012161	29.566	85.952	272.174
<b>CO_Au<sub>15</sub></b>	0.011989	31.261	92.134	293.052
<b>CO_Au<sub>16</sub></b>	0.013097	33.188	97.745	300.679
<b>CO_Au<sub>17</sub></b>	0.012833	34.815	103.988	319.745
<b>CO_Au<sub>18</sub></b>	0.013233	36.618	109.902	333.953
<b>CO_Au<sub>19</sub></b>	0.013278	38.299	116.068	346.976
<b>CO_Au<sub>20</sub></b>	0.013914	40.11	121.91	357.001
<b>CO<sub>2</sub></b>	0.011174	8.676	7.02	51.234
<b>CO<sub>2</sub>_Au<sub>1</sub></b>	0.01128	10.1	12.045	81.684
<b>CO<sub>2</sub>_Au<sub>2</sub></b>	0.011833	11.895	17.911	99.095
<b>CO<sub>2</sub>_Au<sub>3</sub></b>	0.011989	13.675	23.863	124.793
<b>CO<sub>2</sub>_Au<sub>4</sub></b>	0.012713	15.482	29.721	132.735
<b>CO<sub>2</sub>_Au<sub>5</sub></b>	0.013025	17.273	35.631	153.991
<b>CO<sub>2</sub>_Au<sub>6</sub></b>	0.013648	19.082	41.483	165.492
<b>CO<sub>2</sub>_Au<sub>7</sub></b>	0.01394	20.87	47.412	185.177
<b>CO<sub>2</sub>_Au<sub>8</sub></b>	0.01456	22.66	53.28	194.507
<b>CO<sub>2</sub>_Au<sub>9</sub></b>	0.014868	24.455	59.204	213.547
<b>CO<sub>2</sub>_Au<sub>10</sub></b>	0.0152	26.239	65.148	228.834
<b>CO<sub>2</sub>_Au<sub>11</sub></b>	0.015512	28.022	71.072	249.124
<b>CO<sub>2</sub>_Au<sub>12</sub></b>	0.015994	29.808	77.012	256.382

CO <sub>2</sub> _Au <sub>13</sub>	0.016273	30.991	80.983	263.869
CO <sub>2</sub> _Au <sub>14</sub>	0.016851	33.382	88.848	285.216
CO <sub>2</sub> _Au <sub>15</sub>	0.017095	35.16	94.825	299.466
CO <sub>2</sub> _Au <sub>16</sub>	0.017657	36.967	100.682	311.763
CO <sub>2</sub> _Au <sub>17</sub>	0.018093	38.748	106.626	325.789
CO <sub>2</sub> _Au <sub>18</sub>	0.018466	39.943	110.551	331.209
CO <sub>2</sub> _Au <sub>19</sub>	0.019393	42.379	118.296	346.991
CO <sub>2</sub> _Au <sub>20</sub>	0.020147	44.209	124.099	356.115
H <sub>2</sub> O	0.021159	15.057	6.02	45.084
H <sub>2</sub> O_Au <sub>1</sub>	0.022332	16.955	11.509	73.499
H <sub>2</sub> O_Au <sub>2</sub>	0.024136	19.108	16.687	84.689
H <sub>2</sub> O_Au <sub>3</sub>	0.024557	20.358	20.497	103.93
H <sub>2</sub> O_Au <sub>4</sub>	0.025172	22.744	28.398	122.639
H <sub>2</sub> O_Au <sub>5</sub>	0.024508	24.192	34.862	146
H <sub>2</sub> O_Au <sub>6</sub>	0.024744	25.377	38.882	157.856
H <sub>2</sub> O_Au <sub>7</sub>	0.02544	27.682	46.559	176.102
H <sub>2</sub> O_Au <sub>8</sub>	0.026161	29.45	52.268	186.222
H <sub>2</sub> O_Au <sub>9</sub>	0.027059	31.465	57.839	206.943
H <sub>2</sub> O_Au <sub>10</sub>	0.026572	32.996	64.359	219.848
H <sub>2</sub> O_Au <sub>11</sub>	0.0274	34.947	69.98	237.776
H <sub>2</sub> O_Au <sub>12</sub>	0.028829	36.891	74.905	243.148
H <sub>2</sub> O_Au <sub>13</sub>	0.028362	38.514	81.626	259.552
H <sub>2</sub> O_Au <sub>13</sub>	0.027789	38.493	82.16	269.306
H <sub>2</sub> O_Au <sub>14</sub>	0.029337	40.477	87.29	270.206
H <sub>2</sub> O_Au <sub>15</sub>	0.02924	42.189	93.516	290.152
H <sub>2</sub> O_Au <sub>16</sub>	0.030263	44.096	98.907	301.791
H <sub>2</sub> O_Au <sub>17</sub>	0.030002	45.756	105.478	318.383
H <sub>2</sub> O_Au <sub>18</sub>	0.030221	47.401	111.487	329.263
H <sub>2</sub> O_Au <sub>19</sub>	0.030853	49.228	117.367	341.874
H <sub>2</sub> O_Au <sub>20</sub>	0.031675	51.07	123.156	351.134
NO	0.004281	4.168	4.987	49.151
NO_Au <sub>1</sub>	0.003449	4.783	9.811	75.04
NO_Au <sub>2</sub>	0.005484	6.91	13.579	86.905
NO_Au <sub>3</sub>	0.006596	9.075	20.643	101.299
NO_Au <sub>4</sub>	0.006689	11.015	27.163	124.226
NO_Au <sub>5</sub>	0.007278	12.722	32.586	137.189
NO_Au <sub>6</sub>	0.006911	14.619	39.331	163.559
NO_Au <sub>7</sub>	0.007939	15.711	42.414	165.255
NO_Au <sub>8</sub>	0.007897	18.248	51.086	195.644
NO_Au <sub>9</sub>	0.009697	19.958	55.706	194.489
NO_Au <sub>10</sub>	0.008407	21.809	63.012	231.347

NO_Au11	0.01048	23.486	67.61	224.579
NO_Au12	0.009366	24.808	72.813	246.844
NO_Au13	0.011054	27.024	79.577	255.09
NO_Au14	0.010515	28.997	86.528	279.974
NO_Au15	0.011809	30.633	91.472	282.855
NO_Au16	0.009942	31.338	96.547	306.733
NO_Au17	0.012491	34.152	103.383	311.324
NO_Au18	0.011876	36.113	110.29	338.815
NO_Au19	0.01326	37.783	115.395	338.472
NO_Au20	0.013452	39.781	121.909	356.454
NO <sub>2</sub>	0.008122	6.955	7.005	57.577
NO <sub>2</sub> _Au <sub>1</sub>	0.009044	8.012	10.17	71.225
NO <sub>2</sub> _Au <sub>2</sub>	0.009271	9.603	16.377	89.713
NO <sub>2</sub> _Au <sub>3</sub>	0.011038	12.452	23.785	105.593
NO <sub>2</sub> _Au <sub>4</sub>	0.011754	14.353	29.476	123.497
NO <sub>2</sub> _Au <sub>5</sub>	0.011452	15.86	35.768	141.422
NO <sub>2</sub> _Au <sub>6</sub>	0.011688	17.056	39.71	154.101
NO <sub>2</sub> _Au <sub>7</sub>	0.012571	19.516	47.415	173.038
NO <sub>2</sub> _Au <sub>8</sub>	0.012711	21.191	53.317	191.494
NO <sub>2</sub> _Au <sub>9</sub>	0.01414	23.433	58.792	203.838
NO <sub>2</sub> _Au <sub>10</sub>	0.014467	25.21	64.766	217.782
NO <sub>2</sub> _Au <sub>11</sub>	0.013736	26.54	71.141	237.93
NO <sub>2</sub> _Au <sub>12</sub>	0.014162	28.358	77.03	252.112
NO <sub>2</sub> _Au <sub>13</sub>	0.014874	30.212	82.92	264.212
NO <sub>2</sub> _Au <sub>14</sub>	0.01493	31.332	86.905	272.317
NO <sub>2</sub> _Au <sub>15</sub>	0.016546	34.154	94.344	288.979
NO <sub>2</sub> _Au <sub>16</sub>	0.016007	35.521	100.662	305.523
NO <sub>2</sub> _Au <sub>17</sub>	0.01731	37.651	106.299	314.728
NO <sub>2</sub> _Au <sub>18</sub>	0.016695	39.003	112.652	332.896
NO <sub>2</sub> _Au <sub>19</sub>	0.017146	40.802	118.551	343.683
NO <sub>2</sub> _Au <sub>20</sub>	0.018191	42.812	124.385	355.331
SO <sub>2</sub>	0.005698	5.571	8.054	60.249
SO <sub>2</sub> _Au <sub>1</sub>	0.005839	6.358	12.103	76.201
SO <sub>2</sub> _Au <sub>2</sub>	0.007079	8.767	19.642	93.33
SO <sub>2</sub> _Au <sub>3</sub>	0.007686	10.707	25.52	110.416
SO <sub>2</sub> _Au <sub>4</sub>	0.008261	12.314	31.399	120.895
SO <sub>2</sub> _Au <sub>5</sub>	0.008803	14.423	37.14	143.677
SO <sub>2</sub> _Au <sub>6</sub>	0.008615	16.265	43.39	164.921
SO <sub>2</sub> _Au <sub>7</sub>	0.009323	17.935	49.103	177.476
SO <sub>2</sub> _Au <sub>8</sub>	0.009505	19.818	55.187	196.553
SO <sub>2</sub> _Au <sub>9</sub>	0.010465	21.571	60.781	207.362



<b>SO<sub>2</sub>_Au<sub>10</sub></b>	0.011371	23.158	66.591	209.593
<b>SO<sub>2</sub>_Au<sub>11</sub></b>	0.011557	25.161	72.443	235.987
<b>SO<sub>2</sub>_Au<sub>12</sub></b>	0.012037	26.681	78.576	238.233
<b>SO<sub>2</sub>_Au<sub>13</sub></b>	0.011907	28.721	84.447	272.567
<b>SO<sub>2</sub>_Au<sub>14</sub></b>	0.012767	30.23	90.469	269.088
<b>SO<sub>2</sub>_Au<sub>15</sub></b>	0.013441	32.17	96.041	288.409
<b>SO<sub>2</sub>_Au<sub>16</sub></b>	0.013824	33.939	102.053	299.995
<b>SO<sub>2</sub>_Au<sub>17</sub></b>	0.013787	35.211	106.234	311.577
<b>SO<sub>2</sub>_Au<sub>18</sub></b>	0.014056	36.769	112.256	322.698
<b>SO<sub>2</sub>_Au<sub>19</sub></b>	0.014188	39.28	120.309	347.133
<b>SO<sub>2</sub>_Au<sub>20</sub></b>	0.014819	41.325	126.083	361.582

**Table S13**

Adsorption energies obtained for 50 different configurations of SO<sub>2</sub>/Ag<sub>16</sub> complex systems. All calculations were done by M06-2X/SDD method and the values of E<sub>ads</sub> are in kcal/mol

<b>number</b>	<b>E<sub>ads</sub></b>	<b>number</b>	<b>E<sub>ads</sub></b>	<b>number</b>	<b>E<sub>ads</sub></b>	<b>number</b>	<b>E<sub>ads</sub></b>	<b>number</b>	<b>E<sub>ads</sub></b>
<b>1</b>	-106.28	<b>11</b>	-102.71	<b>21</b>	-100.64	<b>31</b>	-97.31	<b>41</b>	-93.67
<b>2</b>	-104.89	<b>12</b>	-102.52	<b>22</b>	-100.38	<b>32</b>	-96.48	<b>42</b>	-93.45
<b>3</b>	-104.89	<b>13</b>	-102.24	<b>23</b>	-100.02	<b>33</b>	-96.48	<b>43</b>	-93.39
<b>4</b>	-104.88	<b>14</b>	-101.75	<b>24</b>	-98.69	<b>34</b>	-95.66	<b>44</b>	-92.02
<b>5</b>	-104.53	<b>15</b>	-101.75	<b>25</b>	-97.62	<b>35</b>	-95.51	<b>45</b>	-91.63
<b>6</b>	-104.39	<b>16</b>	-101.75	<b>26</b>	-97.60	<b>36</b>	-95.21	<b>46</b>	-91.53
<b>7</b>	-103.63	<b>17</b>	-101.75	<b>27</b>	-97.49	<b>37</b>	-94.84	<b>47</b>	-89.73
<b>8</b>	-103.63	<b>18</b>	-101.03	<b>28</b>	-97.43	<b>38</b>	-94.83	<b>48</b>	-89.15
<b>9</b>	-103.35	<b>19</b>	-100.77	<b>29</b>	-97.37	<b>39</b>	-94.51	<b>49</b>	-81.17
<b>10</b>	-103.22	<b>20</b>	-100.71	<b>30</b>	-97.37	<b>40</b>	-94.42	<b>50</b>	-76.92

A number of parameters, including the chemical potential ( $\mu$ ), hardness ( $\eta$ ) [1], and electrophilicity index ( $\omega$ ) [2], which are suitable indicators for predicting the reactivity of species through CDFT can be determined by the information obtained from the electronic structure calculations. These parameters can be predicted as:

$$\mu \cong \frac{(\varepsilon_{LUMO} + \varepsilon_{HOMO})}{2} \quad (1)$$

$$\eta = \frac{1}{2}(IP - EA) \quad (2)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (3)$$

where  $\varepsilon_{HOMO}$  and  $\varepsilon_{LUMO}$  are respectively the HOMO and LUMO energies [3], IP is the Ionization Potential, and EA is Electron Affinity. According to Koopmans' [4] and Janak's [5] approximations, the ionization potential is equal to the negative value of HOMO, ( $\varepsilon_{HOMO} = -IP$ ), and the electron affinity is equal to the negative value of LUMO, ( $\varepsilon_{LUMO} = -EA$ ). The following relation ship is used to obtain the  $\Delta HLG\%$  values,

$$\Delta HLG\% = \frac{HLG_{Complex} - HLG_{Isolated\ cluster}}{HLG_{Isolated\ cluster}} \times 100 \quad (4)$$

In which the  $HLG_{Complex}$  refers to the value of HOMO-LUMO energy gap related to gas/cluster system and  $HLG_{Isolated\ cluster}$  refers to the energy gap of an isolated cluster. This quantity relatively expresses how much the numerical value of the HOMO-LUMO energy gap of gas/cluster systems has changed compared to the isolated clusters.

**Table S14**

Values of electronic total energies (EE) ,in HF, for HOMO energy ( $\varepsilon_{HOMO}$ ), LUMO energy ( $\varepsilon_{LUMO}$ ), HOMO–LUMO energy gap (HLG), chemical potential ( $\mu$ ), chemical hardness ( $\eta$ ), and electrophilicity ( $\omega$ ) from DFT calculations with M06-2X/SDD level of theory for isolated silver clusters, isolated gases, and gas/ $Ag_n$  ( $n=1-22$ ) complex structures. All values are in eV

Name	EE	HOMO	LUMO	HLG	$\Delta HLG\%$	$\eta$	$\mu$	$\omega$
Ag <sub>1</sub>	-146.868	-5.6932	0.1978	5.891	-	2.9455	-2.7477	0.6408
Ag <sub>2</sub>	-293.788	-6.048	-1.9636	4.0844	-	2.0422	-4.0058	1.9643
Ag <sub>3</sub>	-440.68	-4.7304	-2.0403	2.6901	-	1.3451	-3.3854	2.1302
Ag <sub>4</sub>	-587.607	-5.1351	-2.3785	2.7565	-	1.3783	-3.7568	2.56
Ag <sub>5</sub>	-734.528	-5.183	-1.7954	3.3875	-	1.6938	-3.4892	1.7969
Ag <sub>6</sub>	-881.466	-5.8812	-1.8411	4.0401	-	2.02	-3.8612	1.8451
Ag <sub>7</sub>	-1028.39	-4.9696	-1.7886	3.181	-	1.5905	-3.3791	1.7948

Ag <sub>8</sub>	-1175.32	-5.5536	-1.9864	3.5671	-	1.7836	-3.77	1.9922
Ag <sub>9</sub>	-1322.23	-4.9639	-2.0741	2.8899	-	1.4449	-3.519	2.1425
Ag <sub>10</sub>	-1469.16	-4.9059	-2.1913	2.7146	-	1.3573	-3.5486	2.3195
Ag <sub>11</sub>	-1616.08	-4.6268	-2.1062	2.5206	-	1.2603	-3.3665	2.2481
Ag <sub>12</sub>	-1763.02	-5.0757	-2.5111	2.5647	-	1.2823	-3.7934	2.8054
Ag <sub>13</sub>	-1909.94	-4.7225	-2.2819	2.4406	-	1.2203	-3.5022	2.5129
Ag <sub>14</sub>	-2056.88	-5.2948	-2.319	2.9758	-	1.4879	-3.8069	2.435
Ag <sub>15</sub>	-2203.8	-4.8727	-2.3747	2.498	-	1.249	-3.6237	2.6284
Ag <sub>16</sub>	-2350.73	-5.0643	-2.7938	2.2705	-	1.1353	-3.9291	3.3995
Ag <sub>17</sub>	-2497.66	-5.0942	-2.4849	2.6093	-	1.3047	-3.7896	2.7519
Ag <sub>18</sub>	-2644.61	-5.1402	-2.8327	2.3075	-	1.1538	-3.9865	3.4435
Ag <sub>19</sub>	-2791.54	-4.6659	-2.2134	2.4526	-	1.2263	-3.4397	2.412
Ag <sub>20</sub>	-2938.48	-5.0932	-2.258	2.8352	-	1.4176	-3.6756	2.3826
Ag <sub>21</sub>	-3085.39	-4.4055	-2.3799	2.0256	-	1.0128	-3.3927	2.8412
Ag <sub>22</sub>	-3232.32	-4.6812	-2.7799	1.9013	-	0.9506	-3.7305	3.6599
CH <sub>4</sub>	-40.4797	-12.3085	5.5424	17.8509	-	8.9255	-3.3831	0.3206
CH <sub>4</sub> _Ag <sub>1</sub>	-187.35	-5.5772	0.1956	5.7729	2.00475	2.8864	-2.6908	0.6271
CH <sub>4</sub> _Ag <sub>2</sub>	-334.272	-5.8548	-1.6033	4.2515	4.09118	2.1258	-3.729	1.6354
CH <sub>4</sub> _Ag <sub>3</sub>	-481.165	-4.6091	-2.0643	2.5448	5.40129	1.2724	-3.3367	2.1875
CH <sub>4</sub> _Ag <sub>4</sub>	-628.089	-5.0238	-2.3032	2.7206	1.30238	1.3603	-3.6635	2.4666
CH <sub>4</sub> _Ag <sub>5</sub>	-775.012	-5.0872	-1.717	3.3701	0.51365	1.6851	-3.4021	1.7172
CH <sub>4</sub> _Ag <sub>6</sub>	-921.95	-5.7683	-1.6855	4.0828	1.0569	2.0414	-3.7269	1.701
CH <sub>4</sub> _Ag <sub>7</sub>	-1068.87	-4.8749	-1.7538	3.1211	1.88306	1.5606	-3.3143	1.7598
CH <sub>4</sub> _Ag <sub>8</sub>	-1215.81	-5.4638	-1.8893	3.5745	0.20745	1.7872	-3.6765	1.8907
CH <sub>4</sub> _Ag <sub>9</sub>	-1362.71	-4.941	-2.018	2.923	1.14537	1.4615	-3.4795	2.071
CH <sub>4</sub> _Ag <sub>10</sub>	-1509.64	-4.8722	-2.0648	2.8074	3.41855	1.4037	-3.4685	2.1426
CH <sub>4</sub> _Ag <sub>11</sub>	-1656.57	-4.5873	-2.0632	2.5241	0.13886	1.2621	-3.3252	2.1903
CH <sub>4</sub> _Ag <sub>12</sub>	-1803.5	-5.0344	-2.4098	2.6245	2.33166	1.3123	-3.7221	2.6393
CH <sub>4</sub> _Ag <sub>13</sub>	-1950.42	-4.6491	-2.2381	2.4109	1.21691	1.2055	-3.4436	2.4593
CH <sub>4</sub> _Ag <sub>14</sub>	-2097.36	-5.2738	-2.2956	2.9783	0.08401	1.4891	-3.7847	2.4047
CH <sub>4</sub> _Ag <sub>15</sub>	-2244.28	-4.8262	-2.3377	2.4885	0.3803	1.2442	-3.582	2.578
CH <sub>4</sub> _Ag <sub>16</sub>	-2391.21	-5.0126	-2.7511	2.2615	0.39639	1.1308	-3.8818	3.3315
CH <sub>4</sub> _Ag <sub>17</sub>	-2538.14	-5.0398	-2.4441	2.5957	0.52121	1.2978	-3.742	2.6972
CH <sub>4</sub> _Ag <sub>18</sub>	-2685.09	-5.1073	-2.7998	2.3075	0.00433	1.1538	-3.9535	3.3869
CH <sub>4</sub> _Ag <sub>19</sub>	-2832.03	-4.6072	-2.1532	2.4539	0.053	1.227	-3.3802	2.3281
CH <sub>4</sub> _Ag <sub>20</sub>	-2978.97	-5.0676	-2.2308	2.8368	0.05643	1.4184	-3.6492	2.3471

CH <sub>4</sub> _Ag <sub>21</sub>	-3125.88	-4.3832	-2.3652	2.018	0.3752	1.009	-3.3742	2.8209
CH <sub>4</sub> _Ag <sub>22</sub>	-3272.8	-4.6379	-2.7342	1.9037	0.12623	0.9519	-3.6861	3.5686
CO <sub>2</sub>	-188.463	-12.2419	1.0898	13.3317	-	6.6658	-5.576	1.1661
CO <sub>2</sub> _Ag <sub>1</sub>	-335.334	-5.3136	-0.0754	5.2382	11.08131	2.6191	-2.6945	0.693
CO <sub>2</sub> _Ag <sub>2</sub>	-482.259	-5.6913	-1.473	4.2183	3.27833	2.1092	-3.5821	1.5209
CO <sub>2</sub> _Ag <sub>3</sub>	-629.155	-4.3957	-1.6648	2.7309	1.51667	1.3655	-3.0303	1.6812
CO <sub>2</sub> _Ag <sub>4</sub>	-776.083	-5.0104	-1.9845	3.0259	9.77326	1.513	-3.4975	2.0213
CO <sub>2</sub> _Ag <sub>5</sub>	-922.999	-5.1974	-1.7489	3.4485	1.80074	1.7243	-3.4731	1.749
CO <sub>2</sub> _Ag <sub>6</sub>	-1069.94	-5.8815	-1.8351	4.0463	0.15346	2.0232	-3.8583	1.8395
CO <sub>2</sub> _Ag <sub>7</sub>	-1216.86	-4.9761	-1.8036	3.1726	0.26407	1.5863	-3.3899	1.811
CO <sub>2</sub> _Ag <sub>8</sub>	-1363.79	-5.384	-1.8237	3.5603	0.19063	1.7802	-3.6039	1.824
CO <sub>2</sub> _Ag <sub>9</sub>	-1510.7	-4.9478	-2.0368	2.9111	0.73359	1.4555	-3.4923	2.0948
CO <sub>2</sub> _Ag <sub>10</sub>	-1657.63	-4.9051	-2.0893	2.8158	3.72799	1.4079	-3.4972	2.1717
CO <sub>2</sub> _Ag <sub>11</sub>	-1804.55	-5.5868	-2.609	2.9777	18.13457	1.4889	-4.0979	2.8197
CO <sub>2</sub> _Ag <sub>12</sub>	-1951.49	-5.0529	-2.4079	2.6449	3.12707	1.3225	-3.7304	2.6307
CO <sub>2</sub> _Ag <sub>13</sub>	-2098.41	-4.7168	-2.2615	2.4553	0.60231	1.2276	-3.4892	2.4792
CO <sub>2</sub> _Ag <sub>14</sub>	-2245.35	-5.2945	-2.2882	3.0063	1.02493	1.5032	-3.7914	2.3907
CO <sub>2</sub> _Ag <sub>15</sub>	-2392.27	-4.7734	-2.3244	2.449	1.96157	1.2245	-3.5489	2.5714
CO <sub>2</sub> _Ag <sub>16</sub>	-2539.2	-5.0561	-2.7271	2.329	2.57652	1.1645	-3.8916	3.2513
CO <sub>2</sub> _Ag <sub>17</sub>	-2686.13	-5.0831	-2.4762	2.6069	0.09198	1.3034	-3.7797	2.7401
CO <sub>2</sub> _Ag <sub>18</sub>	-2833.08	-5.0864	-2.7941	2.2923	0.65872	1.1461	-3.9402	3.3864
CO <sub>2</sub> _Ag <sub>19</sub>	-2980.01	-4.6697	-2.1894	2.4803	1.12941	1.2402	-3.4296	2.3711
CO <sub>2</sub> _Ag <sub>20</sub>	-3126.96	-5.1849	-2.1611	3.0237	6.64856	1.5119	-3.673	2.2308
CO <sub>2</sub> _Ag <sub>21</sub>	-3273.87	-4.4205	-2.3818	2.0387	0.64672	1.0193	-3.4012	2.8371
CO <sub>2</sub> _Ag <sub>22</sub>	-3420.79	-4.6719	-2.7666	1.9053	0.21038	0.9527	-3.7193	3.63
CO	-113.236	-12.1512	0.034	12.1853	-	6.0926	-6.0586	1.5062
CO_Ag <sub>1</sub>	-260.111	-5.3947	-0.8504	4.5443	22.8603	2.2722	-3.1225	1.0728
CO_Ag <sub>2</sub>	-407.031	-5.7574	-1.4289	4.3285	5.9764	2.1643	-3.5931	1.4913
CO_Ag <sub>3</sub>	-553.936	-5.3231	-1.5257	3.7974	41.16204	1.8987	-3.4244	1.5441
CO_Ag <sub>4</sub>	-700.87	-5.1465	-1.6468	3.4997	26.96173	1.7498	-3.3967	1.6483
CO_Ag <sub>5</sub>	-847.776	-4.9272	-1.83	3.0972	8.56974	1.5486	-3.3786	1.8427
CO_Ag <sub>6</sub>	-994.712	-5.6469	-1.8711	3.7759	6.53944	1.8879	-3.759	1.8711
CO_Ag <sub>7</sub>	-1141.64	-4.8273	-1.8202	3.0071	5.46683	1.5036	-3.3237	1.8368
CO_Ag <sub>8</sub>	-1288.57	-5.3941	-1.9687	3.4254	3.97241	1.7127	-3.6814	1.9783
CO_Ag <sub>9</sub>	-1435.48	-4.8828	-2.0618	2.821	2.38417	1.4105	-3.4723	2.137
CO_Ag <sub>10</sub>	-1582.41	-4.9348	-2.0732	2.8616	5.41516	1.4308	-3.504	2.1454

CO_Ag11	-1729.33	-4.5892	-2.0868	2.5024	0.72205	1.2512	-3.338	2.2264
CO_Ag12	-1876.27	-4.9854	-2.556	2.4294	5.27547	1.2147	-3.7707	2.9262
CO_Ag13	-2023.18	-4.6042	-2.2068	2.3973	1.77415	1.1987	-3.4055	2.4188
CO_Ag14	-2170.14	-5.2464	-2.4395	2.8069	5.67578	1.4034	-3.8429	2.6307
CO_Ag15	-2317.04	-4.7729	-2.3165	2.4564	1.66533	1.2282	-3.5447	2.5576
CO_Ag16	-2463.97	-4.9751	-2.7236	2.2515	0.83682	1.1257	-3.8493	3.2906
CO_Ag17	-2610.9	-5.0298	-2.4248	2.6049	0.16863	1.3025	-3.7273	2.6666
CO_Ag18	-2757.86	-5.1503	-2.7018	2.4485	6.11051	1.2242	-3.9261	3.1477
CO_Ag19	-2904.78	-4.5702	-2.1818	2.3883	2.62171	1.1942	-3.376	2.386
CO_Ag20	-3051.73	-5.0659	-2.2425	2.8235	0.41267	1.4117	-3.6542	2.3647
CO_Ag21	-3198.64	-4.377	-2.3508	2.0262	0.02962	1.0131	-3.3639	2.7924
CO_Ag22	-3345.57	-4.6099	-2.7413	1.8686	1.71988	0.9343	-3.6756	3.615
H <sub>2</sub> O	-76.3795	-10.4633	3.3206	13.7839	-	6.892	-3.5714	0.4627
H <sub>2</sub> O_Ag1	-223.26	-4.5636	-0.1156	4.448	24.49499	2.224	-2.3396	0.6153
H <sub>2</sub> O_Ag2	-370.191	-5.279	-1.1848	4.0942	0.23994	2.0471	-3.2319	1.2756
H <sub>2</sub> O_Ag3	-517.089	-4.067	-1.3845	2.6825	0.28252	1.3412	-2.7258	1.3849
H <sub>2</sub> O_Ag4	-664.018	-4.7576	-1.8207	2.9369	6.54453	1.4685	-3.2892	1.8418
H <sub>2</sub> O_Ag5	-810.928	-4.6545	-1.4085	3.246	4.17712	1.623	-3.0315	1.4156
H <sub>2</sub> O_Ag6	-957.865	-5.4551	-1.6251	3.83	5.20037	1.915	-3.5401	1.636
H <sub>2</sub> O_Ag7	-1104.79	-4.5707	-1.9026	2.6681	16.12386	1.334	-3.2367	1.9632
H <sub>2</sub> O_Ag8	-1251.72	-5.1917	-2.0123	3.1794	10.86877	1.5897	-3.602	2.0404
H <sub>2</sub> O_Ag9	-1398.63	-4.7944	-1.9364	2.858	1.10384	1.429	-3.3654	1.9814
H <sub>2</sub> O_Ag10	-1545.56	-4.9732	-2.0139	2.9592	9.01054	1.4796	-3.4935	2.0621
H <sub>2</sub> O_Ag11	-1692.48	-4.4167	-1.9013	2.5154	0.2063	1.2577	-3.159	1.9836
H <sub>2</sub> O_Ag12	-1839.42	-4.8964	-2.5013	2.3951	6.61286	1.1976	-3.6988	2.8561
H <sub>2</sub> O_Ag13	-1986.34	-4.504	-2.3821	2.1219	13.05826	1.061	-3.4431	2.7933
H <sub>2</sub> O_Ag14	-2133.28	-5.1127	-2.1897	2.923	1.77431	1.4615	-3.6512	2.2804
H <sub>2</sub> O_Ag15	-2280.2	-4.5854	-2.2006	2.3848	4.53163	1.1924	-3.393	2.4137
H <sub>2</sub> O_Ag16	-2427.13	-4.8989	-2.5383	2.3606	3.96829	1.1803	-3.7186	2.9289
H <sub>2</sub> O_Ag17	-2574.06	-4.6404	-2.3981	2.2422	14.06891	1.1211	-3.5192	2.7618
H <sub>2</sub> O_Ag18	-2721.01	-4.8736	-2.5165	2.3571	2.14951	1.1785	-3.695	2.8963
H <sub>2</sub> O_Ag19	-2867.94	-4.4902	-2.2068	2.2833	6.90288	1.1417	-3.3485	2.4553
H <sub>2</sub> O_Ag20	-3014.89	-4.9307	-2.2618	2.6689	5.86555	1.3344	-3.5963	2.4229
H <sub>2</sub> O_Ag21	-3161.79	-4.3408	-2.3372	2.0036	1.0861	1.0018	-3.339	2.7822
H <sub>2</sub> O_Ag22	-3308.72	-4.6352	-2.756	1.8792	1.16236	0.9396	-3.6956	3.6338
NO <sub>2</sub>	-204.939	-10.561	-2.1761	8.3849	-	4.1925	-6.3686	2.4185

NO <sub>2</sub> _Ag <sub>1</sub>	-351.895	-8.9204	-2.7372	6.1832	4.96011	3.0916	-5.8288	2.7474
NO <sub>2</sub> _Ag <sub>2</sub>	-498.788	-7.7103	-2.0917	5.6186	37.56243	2.8093	-4.901	2.1376
NO <sub>2</sub> _Ag <sub>3</sub>	-645.744	-6.8113	-2.1701	4.6412	72.5289	2.3206	-4.4907	2.1725
NO <sub>2</sub> _Ag <sub>4</sub>	-792.651	-5.8578	-1.9399	3.9179	42.13314	1.9589	-3.8988	1.9399
NO <sub>2</sub> _Ag <sub>5</sub>	-939.59	-6.3133	-2.6341	3.6793	8.61402	1.8396	-4.4737	2.7198
NO <sub>2</sub> _Ag <sub>6</sub>	-1086.5	-5.2523	-2.4215	2.8308	29.93243	1.4154	-3.8369	2.6003
NO <sub>2</sub> _Ag <sub>7</sub>	-1233.42	-6.0012	-2.4703	3.531	11.00283	1.7655	-4.2357	2.5406
NO <sub>2</sub> _Ag <sub>8</sub>	-1380.35	-5.7574	-2.3356	3.4218	4.07334	1.7109	-4.0465	2.3926
NO <sub>2</sub> _Ag <sub>9</sub>	-1527.26	-5.3702	-2.6428	2.7274	5.62303	1.3637	-4.0065	2.9427
NO <sub>2</sub> _Ag <sub>10</sub>	-1674.2	-4.9451	-2.4387	2.5064	7.66964	1.2532	-3.6919	2.719
NO <sub>2</sub> _Ag <sub>11</sub>	-1821.12	-5.5911	-2.6632	2.9279	16.15885	1.464	-4.1272	2.9088
NO <sub>2</sub> _Ag <sub>12</sub>	-1968.05	-5.1762	-2.7119	2.4643	3.91469	1.2321	-3.944	3.1562
NO <sub>2</sub> _Ag <sub>13</sub>	-2114.98	-5.5732	-2.9865	2.5867	5.98623	1.2934	-4.2798	3.5405
NO <sub>2</sub> _Ag <sub>14</sub>	-2261.91	-5.1985	-2.5285	2.67	10.27623	1.335	-3.8635	2.7952
NO <sub>2</sub> _Ag <sub>15</sub>	-2408.84	-5.5171	-2.7666	2.7505	10.10809	1.3753	-4.1418	3.1185
NO <sub>2</sub> _Ag <sub>16</sub>	-2555.77	-4.778	-2.5552	2.2229	2.09645	1.1114	-3.6666	3.024
NO <sub>2</sub> _Ag <sub>17</sub>	-2702.71	-5.2031	-2.8485	2.3546	9.76124	1.1773	-4.0258	3.4416
NO <sub>2</sub> _Ag <sub>18</sub>	-2849.63	-5.2937	-2.9786	2.3151	0.32936	1.1576	-4.1361	3.6947
NO <sub>2</sub> _Ag <sub>19</sub>	-2996.58	-5.051	-2.9598	2.0912	14.73538	1.0456	-4.0054	3.8359
NO <sub>2</sub> _Ag <sub>20</sub>	-3143.51	-5.2673	-2.4243	2.843	0.27511	1.4215	-3.8458	2.6011
NO <sub>2</sub> _Ag <sub>21</sub>	-3290.44	-5.0942	-2.6781	2.4161	19.27824	1.208	-3.8862	3.1254
NO <sub>2</sub> _Ag <sub>22</sub>	-3437.37	-4.7054	-2.676	2.0294	6.7375	1.0147	-3.6907	3.3559
NO	-129.807	-8.647	-1.996	6.651	-	3.3255	-5.3215	2.1288
NO_Ag <sub>1</sub>	-276.679	-6.2227	-2.2281	3.9946	32.19148	1.9973	-4.2254	2.2347
NO_Ag <sub>2</sub>	-423.603	-5.8151	-3.0403	2.7747	32.06591	1.3874	-4.4277	3.5327
NO_Ag <sub>3</sub>	-570.519	-6.34	-1.9296	4.4104	63.9493	2.2052	-4.1348	1.9382
NO_Ag <sub>4</sub>	-717.433	-5.4123	-2.6218	2.7905	1.23345	1.3953	-4.0171	2.8914
NO_Ag <sub>5</sub>	-864.342	-5.9705	-2.273	3.6975	9.15129	1.8487	-4.1217	2.2973
NO_Ag <sub>6</sub>	-1011.28	-5.8543	-2.2629	3.5914	11.10616	1.7957	-4.0586	2.2933
NO_Ag <sub>7</sub>	-1158.21	-5.5509	-2.3209	3.23	1.5404	1.615	-3.9359	2.398
NO_Ag <sub>8</sub>	-1305.14	-5.3704	-2.7489	2.6215	26.50893	1.3108	-4.0597	3.1434
NO_Ag <sub>9</sub>	-1452.07	-5.6695	-2.2373	3.4322	18.76536	1.7161	-3.9534	2.2769
NO_Ag <sub>10</sub>	-1599	-5.9615	-2.6931	3.2684	20.4008	1.6342	-4.3273	2.8647
NO_Ag <sub>11</sub>	-1745.92	-5.4695	-2.4245	3.045	20.80457	1.5225	-3.947	2.5582
NO_Ag <sub>12</sub>	-1892.85	-5.3432	-2.8673	2.476	3.45849	1.238	-4.1052	3.4033
NO_Ag <sub>13</sub>	-2039.76	-5.393	-3.2096	2.1834	10.53839	1.0917	-4.3013	4.2367

NO_Ag14	-2186.7	-5.346	-2.5856	2.7603	7.24175	1.3802	-3.9658	2.8488
NO_Ag15	-2333.62	-5.3906	-2.8512	2.5394	1.65733	1.2697	-4.1209	3.3437
NO_Ag16	-2480.57	-5.3163	-2.8381	2.4781	9.14336	1.2391	-4.0772	3.3541
NO_Ag17	-2627.48	-5.2428	-2.8082	2.4346	6.69528	1.2173	-4.0255	3.328
NO_Ag18	-2774.43	-5.1182	-2.8469	2.2713	1.5688	1.1357	-3.9825	3.4914
NO_Ag19	-2921.36	-4.9111	-2.8664	2.0447	16.63133	1.0223	-3.8888	3.6981
NO_Ag20	-3068.3	-5.0844	-2.7671	2.3173	18.26679	1.1587	-3.9258	3.3253
NO_Ag21	-3215.21	-5.0608	-2.762	2.2988	13.48736	1.1494	-3.9114	3.3275
NO_Ag22	-3362.14	-4.8902	-2.6088	2.2814	19.99158	1.1407	-3.7495	3.0811
SO <sub>2</sub>	-548.358	-11.1368	-4.1005	7.0363	-	3.5182	-7.6186	4.1246
SO <sub>2</sub> _Ag1	-695.324	-7.654	-2.4112	5.2428	11.00323	2.6214	-5.0326	2.4154
SO <sub>2</sub> _Ag2	-989.183	-6.7528	-1.9298	4.8229	18.08099	2.4115	-4.3413	1.9539
SO <sub>2</sub> _Ag3	-1136.1	-5.9141	-2.2436	3.6705	36.44474	1.8353	-4.0789	2.2663
SO <sub>2</sub> _Ag4	-1282.99	-5.6613	-2.9854	2.676	2.92037	1.338	-4.3233	3.4924
SO <sub>2</sub> _Ag5	-1429.96	-6.0352	-2.3617	3.6735	8.4428	1.8368	-4.1984	2.3992
SO <sub>2</sub> _Ag6	-1576.87	-5.6766	-2.1274	3.5492	12.15069	1.7746	-3.902	2.1449
SO <sub>2</sub> _Ag7	-1723.81	-5.6461	-2.3418	3.3043	3.87614	1.6521	-3.994	2.4138
SO <sub>2</sub> _Ag8	-1870.73	-5.6907	-2.1263	3.5644	0.07569	1.7822	-3.9085	2.1429
SO <sub>2</sub> _Ag9	-2017.67	-5.6945	-2.4526	3.242	12.18381	1.621	-4.0735	2.5592
SO <sub>2</sub> _Ag10	-2164.58	-5.2981	-2.2847	3.0134	11.00715	1.5067	-3.7914	2.3851
SO <sub>2</sub> _Ag11	-2311.53	-5.525	-2.3943	3.1307	24.20455	1.5653	-3.9597	2.5041
SO <sub>2</sub> _Ag12	-2458.42	-5.0458	-2.679	2.3668	7.7163	1.1834	-3.8624	3.1515
SO <sub>2</sub> _Ag13	-2605.39	-5.3503	-2.8118	2.5386	4.01541	1.2693	-4.081	3.2804
SO <sub>2</sub> _Ag14	-2752.3	-5.1631	-2.6014	2.5617	13.91559	1.2808	-3.8822	2.9418
SO <sub>2</sub> _Ag15	-2899.24	-5.3201	-2.8229	2.4972	0.03203	1.2486	-4.0715	3.3192
SO <sub>2</sub> _Ag16	-3046.14	-5.128	-3.4795	1.6485	27.39485	0.8242	-4.3038	5.618
SO <sub>2</sub> _Ag17	-3193.11	-5.4159	-3.0216	2.3943	8.23976	1.1972	-4.2187	3.7166
SO <sub>2</sub> _Ag18	-3340.04	-4.8502	-2.476	2.3742	2.89057	1.1871	-3.6631	2.8258
SO <sub>2</sub> _Ag19	-3486.98	-5.4074	-2.723	2.6844	9.45119	1.3422	-4.0652	3.0782
SO <sub>2</sub> _Ag20	-3633.88	-5.0148	-2.5807	2.4341	14.14715	1.217	-3.7978	2.9627
SO <sub>2</sub> _Ag21	-3780.82	-5.0744	-2.9922	2.0822	2.79423	1.0411	-4.0333	3.9062
SO <sub>2</sub> _Ag22	-842.176	-6.4635	-3.4899	2.9737	56.40351	1.4868	-4.9767	4.1645

**Table S15**

Values of electronic total energies (EE) ,in HF, for HOMO energy ( $\epsilon_{\text{HOMO}}$ ), LUMO energy ( $\epsilon_{\text{LUMO}}$ ), HOMO–LUMO energy gap (HLG), chemical potential ( $\mu$ ), chemical hardness ( $\eta$ ), and electrophilicity ( $\omega$ ) from DFT calculations with M06-2X/SDD level of theory for isolated gold clusters, isolated gases, and gas/Au<sub>n</sub> (n=1-20) complex structures. All values are in eV

Name	EE	HOMO	LUMO	HLG	$\Delta$ HLG%	$\eta$	$\mu$	$\omega$
Au <sub>1</sub>	-135.599	-7.4203	0.0454	7.4657	-	3.7329	-3.6874	0.9106
Au <sub>2</sub>	-271.251	-7.5297	-2.676	4.8537	-	2.4268	-5.1028	2.6824
Au <sub>3</sub>	-406.877	-7.3822	-2.0917	5.2904	-	2.6452	-4.737	2.1207
Au <sub>4</sub>	-542.535	-6.4031	-3.0504	3.3527	-	1.6764	-4.7268	3.332
Au <sub>5</sub>	-678.193	-6.3979	-2.2781	4.1198	-	2.0599	-4.338	2.2839
Au <sub>6</sub>	-813.877	-7.4099	-2.2893	5.1206	-	2.5603	-4.8496	2.2965
Au <sub>7</sub>	-949.511	-6.3408	-2.4011	3.9397	-	1.9698	-4.371	2.4247
Au <sub>8</sub>	-1085.19	-6.9629	-2.7905	4.1723	-	2.0862	-4.8767	2.85
Au <sub>9</sub>	-1220.82	-6.2605	-2.8137	3.4469	-	1.7234	-4.5371	2.9861
Au <sub>10</sub>	-1356.49	-6.4831	-2.9309	3.5522	-	1.7761	-4.707	3.1187
Au <sub>11</sub>	-1492.13	-6.2782	-2.8915	3.3867	-	1.6934	-4.5848	3.1034
Au <sub>12</sub>	-1627.82	-6.4924	-2.9726	3.5198	-	1.7599	-4.7325	3.1815
Au <sub>13</sub>	-1763.47	-6.1767	-2.6458	3.531	-	1.7655	-4.4112	2.7555
Au <sub>14</sub>	-1899.14	-6.5566	-2.7971	3.7595	-	1.8798	-4.6768	2.909
Au <sub>15</sub>	-2034.79	-5.891	-2.8877	3.0033	-	1.5017	-4.3893	3.2075
Au <sub>16</sub>	-2170.46	-6.1661	-3.2186	2.9475	-	1.4738	-4.6923	3.735
Au <sub>17</sub>	-2306.13	-5.977	-2.6795	3.2975	-	1.6487	-4.3282	2.8406
Au <sub>18</sub>	-2441.8	-6.3356	-3.1647	3.1709	-	1.5855	-4.7502	3.5579
Au <sub>19</sub>	-2577.49	-5.7792	-2.4839	3.2953	-	1.6477	-4.1315	2.59
Au <sub>20</sub>	-2713.18	-6.9283	-2.4384	4.4899	-	2.2449	-4.6834	2.4426
CH <sub>4</sub>	-40.4797	-12.3113	5.5242	17.8354	-	8.9177	-3.3935	0.3228
CH <sub>4</sub> _Au <sub>1</sub>	-176.081	-7.281	0.012	7.2929	2.31459	3.6465	-3.6345	0.9056
CH <sub>4</sub> _Au <sub>2</sub>	-311.738	-7.3016	-2.0381	5.2635	8.44304	2.6318	-4.6699	2.0716
CH <sub>4</sub> _Au <sub>3</sub>	-447.362	-5.6744	-2.3108	3.3636	36.42069	1.6818	-3.9926	2.3696
CH <sub>4</sub> _Au <sub>4</sub>	-583.023	-6.2418	-2.7386	3.5032	4.48892	1.7516	-4.4902	2.8776
CH <sub>4</sub> _Au <sub>5</sub>	-718.677	-6.3816	-2.2624	4.1193	0.01214	2.0596	-4.322	2.2673
CH <sub>4</sub> _Au <sub>6</sub>	-854.362	-7.3942	-2.2702	5.1239	0.06445	2.562	-4.8322	2.2786
CH <sub>4</sub> _Au <sub>7</sub>	-989.996	-6.3424	-2.3394	4.0031	1.60926	2.0015	-4.3409	2.3536



<b>CH<sub>4</sub>_Au<sub>8</sub></b>	-1125.67	-6.9601	-2.6645	4.2956	2.9552	2.1478	-4.8123	2.6956
<b>CH<sub>4</sub>_Au<sub>9</sub></b>	-1261.31	-6.2382	-2.7285	3.5097	1.82193	1.7549	-4.4833	2.8635
<b>CH<sub>4</sub>_Au<sub>10</sub></b>	-1396.97	-6.4782	-2.8414	3.6368	2.38162	1.8184	-4.6598	2.9853
<b>CH<sub>4</sub>_Au<sub>11</sub></b>	-1532.62	-6.2548	-2.839	3.4158	0.85924	1.7079	-4.5469	3.0262
<b>CH<sub>4</sub>_Au<sub>12</sub></b>	-1668.31	-6.4698	-2.845	3.6248	2.98312	1.8124	-4.6574	2.992
<b>CH<sub>4</sub>_Au<sub>13</sub></b>	-1803.95	-6.1509	-2.6539	3.4969	0.96573	1.7485	-4.4024	2.7712
<b>CH<sub>4</sub>_Au<sub>14</sub></b>	-1939.63	-6.519	-2.7647	3.7544	0.13566	1.8772	-4.6419	2.8696
<b>CH<sub>4</sub>_Au<sub>15</sub></b>	-2075.27	-5.8651	-2.8033	3.0618	1.94786	1.5309	-4.3342	3.0677
<b>CH<sub>4</sub>_Au<sub>16</sub></b>	-2210.95	-6.1408	-3.1805	2.9603	0.43427	1.4802	-4.6606	3.6688
<b>CH<sub>4</sub>_Au<sub>17</sub></b>	-2346.61	-5.9579	-2.6338	3.3241	0.80667	1.6621	-4.2959	2.7758
<b>CH<sub>4</sub>_Au<sub>18</sub></b>	-2482.28	-6.2951	-3.1339	3.1611	0.30906	1.5806	-4.7145	3.5156
<b>CH<sub>4</sub>_Au<sub>19</sub></b>	-2617.97	-5.7446	-2.4705	3.2741	0.64334	1.637	-4.1076	2.5766
<b>CH<sub>4</sub>_Au<sub>20</sub></b>	-2753.67	-6.9049	-2.4316	4.4733	0.36972	2.2366	-4.6683	2.4359
<b>CO<sub>2</sub></b>	-188.463	-12.2419	0.8904	13.1322	-	6.5661	-5.6758	1.2265
<b>CO<sub>2</sub>_Au<sub>1</sub></b>	-324.065	-7.6323	-0.0895	7.5427	1.03138	3.7714	-3.8609	0.9881
<b>CO<sub>2</sub>_Au<sub>2</sub></b>	-459.72	-7.5776	-1.7807	5.7968	19.43054	2.8984	-4.6791	1.8885
<b>CO<sub>2</sub>_Au<sub>3</sub></b>	-595.347	-7.0548	-2.1277	4.9272	6.86527	2.4636	-4.5912	2.1391
<b>CO<sub>2</sub>_Au<sub>4</sub></b>	-731.008	-6.4747	-3.1816	3.2931	1.77767	1.6466	-4.8281	3.5393
<b>CO<sub>2</sub>_Au<sub>5</sub></b>	-866.664	-6.3822	-2.384	3.9982	2.9516	1.9991	-4.3831	2.4025
<b>CO<sub>2</sub>_Au<sub>6</sub></b>	-1002.35	-7.4254	-2.2702	5.1552	0.6757	2.5776	-4.8478	2.2794
<b>CO<sub>2</sub>_Au<sub>7</sub></b>	-1137.98	-6.3283	-2.3421	3.9862	1.18029	1.9931	-4.3352	2.3574
<b>CO<sub>2</sub>_Au<sub>8</sub></b>	-1273.66	-7.0907	-2.7511	4.3397	4.01218	2.1698	-4.9209	2.79
<b>CO<sub>2</sub>_Au<sub>9</sub></b>	-1409.29	-6.2671	-2.7666	3.5005	1.55502	1.7502	-4.5168	2.9141
<b>CO<sub>2</sub>_Au<sub>10</sub></b>	-1544.96	-6.4774	-2.8675	3.6099	1.62435	1.8049	-4.6725	3.0239
<b>CO<sub>2</sub>_Au<sub>11</sub></b>	-1680.61	-6.2798	-2.8749	3.405	0.54035	1.7025	-4.5774	3.0767
<b>CO<sub>2</sub>_Au<sub>12</sub></b>	-1816.29	-6.5062	-2.9655	3.5407	0.59378	1.7704	-4.7359	3.1672
<b>CO<sub>2</sub>_Au<sub>13</sub></b>	-1951.94	-6.1816	-2.6689	3.5127	0.51827	1.7564	-4.4253	2.7874
<b>CO<sub>2</sub>_Au<sub>14</sub></b>	-2087.62	-6.5656	-2.7821	3.7835	0.63838	1.8917	-4.6738	2.8869
<b>CO<sub>2</sub>_Au<sub>15</sub></b>	-2223.26	-5.8358	-2.9143	2.9214	2.727	1.4607	-4.375	3.276
<b>CO<sub>2</sub>_Au<sub>16</sub></b>	-2358.94	-6.2007	-3.2088	2.9919	1.50636	1.4959	-4.7047	3.6991
<b>CO<sub>2</sub>_Au<sub>17</sub></b>	-2494.6	-5.9808	-2.6762	3.3046	0.21531	1.6523	-4.3285	2.8349
<b>CO<sub>2</sub>_Au<sub>18</sub></b>	-2630.27	-6.3541	-3.1905	3.1636	0.23022	1.5818	-4.7723	3.5996
<b>CO<sub>2</sub>_Au<sub>19</sub></b>	-2765.96	-5.7585	-2.4828	3.2757	0.59479	1.6379	-4.1206	2.5917
<b>CO<sub>2</sub>_Au<sub>20</sub></b>	-2901.65	-6.9294	-2.4444	4.485	0.10913	2.2425	-4.6869	2.4489

<b>CO</b>	-113.236	-12.151	-0.0873	12.0636	-	6.0318	-6.1192	1.5519
<b>CO_Au<sub>1</sub></b>	-248.846	-6.7351	-0.948	5.787	22.4855	2.8935	-3.8416	1.2751
<b>CO_Au<sub>2</sub></b>	-384.525	-7.2423	-2.3116	4.9307	1.58642	2.4654	-4.777	2.314
<b>CO_Au<sub>3</sub></b>	-520.154	-5.716	-1.7399	3.9761	24.84311	1.9881	-3.728	1.7476
<b>CO_Au<sub>4</sub></b>	-655.816	-6.4222	-2.0422	4.3799	30.63799	2.19	-4.2322	2.0447
<b>CO_Au<sub>5</sub></b>	-791.437	-6.4072	-2.2858	4.1214	0.03884	2.0607	-4.3465	2.2919
<b>CO_Au<sub>6</sub></b>	-927.122	-7.4034	-2.3043	5.0991	0.41987	2.5496	-4.8538	2.3102
<b>CO_Au<sub>7</sub></b>	-1062.76	-6.3511	-2.4017	3.9495	0.24875	1.9747	-4.3764	2.4248
<b>CO_Au<sub>8</sub></b>	-1198.43	-6.9819	-2.6847	4.2972	2.99355	2.1486	-4.8333	2.7181
<b>CO_Au<sub>9</sub></b>	-1334.07	-5.943	-2.7113	3.2316	6.24619	1.6158	-4.3272	2.897
<b>CO_Au<sub>10</sub></b>	-1469.73	-6.488	-2.9353	3.5527	0.01408	1.7764	-4.7117	3.1243
<b>CO_Au<sub>11</sub></b>	-1605.38	-6.2834	-2.8498	3.4335	1.38188	1.7168	-4.5666	3.0368
<b>CO_Au<sub>12</sub></b>	-1741.08	-6.3808	-2.7187	3.6621	4.04284	1.8311	-4.5497	2.8263
<b>CO_Au<sub>13</sub></b>	-1876.73	-5.9337	-2.5971	3.3367	5.50269	1.6683	-4.2654	2.7263
<b>CO_Au<sub>14</sub></b>	-2012.41	-6.4042	-2.7451	3.6591	2.67057	1.8296	-4.5746	2.8596
<b>CO_Au<sub>15</sub></b>	-2148.05	-5.6224	-2.8662	2.7562	8.22762	1.3781	-4.2443	3.2679
<b>CO_Au<sub>16</sub></b>	-2283.74	-6.1677	-3.0052	3.1625	7.29432	1.5813	-4.5865	3.3258
<b>CO_Au<sub>17</sub></b>	-2419.38	-5.6744	-2.6855	2.9889	9.35861	1.4944	-4.1799	2.9228
<b>CO_Au<sub>18</sub></b>	-2555.05	-6.0671	-3.1514	2.9157	8.04819	1.4579	-4.6092	3.6432
<b>CO_Au<sub>19</sub></b>	-2690.73	-5.7416	-2.4939	3.2477	1.44448	1.6238	-4.1178	2.6105
<b>CO_Au<sub>20</sub></b>	-2826.43	-6.9019	-2.4479	4.454	0.79957	2.227	-4.6749	2.4534
<b>H<sub>2</sub>O</b>	-76.3795	-10.4633	3.3206	13.7839	-	6.892	-3.5714	0.4627
<b>H<sub>2</sub>O_Au<sub>1</sub></b>	-211.99	-6.0962	-0.169	5.9272	20.60758	2.9636	-3.1326	0.8278
<b>H<sub>2</sub>O_Au<sub>2</sub></b>	-347.661	-6.7302	-1.4417	5.2885	8.95811	2.6443	-4.0859	1.5784
<b>H<sub>2</sub>O_Au<sub>3</sub></b>	-483.287	-5.2793	-1.7753	3.504	33.76682	1.752	-3.5273	1.7753
<b>H<sub>2</sub>O_Au<sub>4</sub></b>	-618.948	-5.8782	-1.9949	3.8833	15.82605	1.9417	-3.9365	1.9952
<b>H<sub>2</sub>O_Au<sub>5</sub></b>	-754.589	-5.6875	-1.8838	3.8036	7.67513	1.9018	-3.7856	1.8839
<b>H<sub>2</sub>O_Au<sub>6</sub></b>	-890.272	-6.8333	-2.1037	4.7296	7.63582	2.3648	-4.4685	2.1109
<b>H<sub>2</sub>O_Au<sub>7</sub></b>	-1025.91	-6.3786	-2.2722	4.1065	4.23382	2.0532	-4.3254	2.278
<b>H<sub>2</sub>O_Au<sub>8</sub></b>	-1161.58	-7.0513	-2.5862	4.4651	7.01771	2.2326	-4.8187	2.6002
<b>H<sub>2</sub>O_Au<sub>9</sub></b>	-1297.22	-5.94	-2.6044	3.3356	3.22899	1.6678	-4.2722	2.7359
<b>H<sub>2</sub>O_Au<sub>10</sub></b>	-1432.88	-6.479	-2.7527	3.7263	4.90119	1.8632	-4.6159	2.8589
<b>H<sub>2</sub>O_Au<sub>11</sub></b>	-1568.53	-6.0439	-2.7228	3.3212	1.93404	1.6606	-4.3833	2.8926
<b>H<sub>2</sub>O_Au<sub>12</sub></b>	-1704.23	-6.3351	-2.7886	3.5465	0.75857	1.7732	-4.5619	2.934

H <sub>2</sub> O_Au <sub>13</sub>	-1839.86	-5.7843	-2.4507	3.3337	5.58765	1.6668	-4.1175	2.5428
H <sub>2</sub> O_Au <sub>14</sub>	-1975.55	-6.146	-2.603	3.5429	5.7614	1.7715	-4.3745	2.7006
H <sub>2</sub> O_Au <sub>15</sub>	-2111.19	-5.6047	-2.7097	2.895	3.60603	1.4475	-4.1572	2.9849
H <sub>2</sub> O_Au <sub>16</sub>	-2246.87	-6.0706	-2.9133	3.1573	7.1179	1.5787	-4.4919	3.1953
H <sub>2</sub> O_Au <sub>17</sub>	-2382.53	-5.7666	-2.4134	3.3533	1.69219	1.6766	-4.09	2.4943
H <sub>2</sub> O_Au <sub>18</sub>	-2518.19	-6.2023	-3.0371	3.1652	0.17976	1.5826	-4.6197	3.3712
H <sub>2</sub> O_Au <sub>19</sub>	-2653.88	-5.6632	-2.3573	3.3059	0.32167	1.653	-4.0103	2.4324
H <sub>2</sub> O_Au <sub>20</sub>	-2789.58	-6.8143	-2.399	4.4153	1.66151	2.2077	-4.6066	2.4031
NO <sub>2</sub>	-204.939	-10.5561	-2.4433	8.1128	-	4.0564	-6.4997	2.6037
NO <sub>2</sub> _Au <sub>1</sub>	-340.592	-9.4745	-3.2912	6.1832	17.17856	3.0916	-6.3828	3.2944
NO <sub>2</sub> _Au <sub>2</sub>	-476.223	-7.2736	-3.0469	4.2267	12.91798	2.1134	-5.1602	3.1499
NO <sub>2</sub> _Au <sub>3</sub>	-611.899	-8.1974	-3.0792	5.1182	3.25495	2.5591	-5.6383	3.1057
NO <sub>2</sub> _Au <sub>4</sub>	-747.548	-7.2956	-2.4308	4.8649	45.10395	2.4324	-4.8632	2.4308
NO <sub>2</sub> _Au <sub>5</sub>	-883.228	-7.9348	-2.6588	5.276	28.06447	2.638	-5.2968	2.6589
NO <sub>2</sub> _Au <sub>6</sub>	-1018.86	-7.1375	-2.5489	4.5887	10.38745	2.2943	-4.8432	2.556
NO <sub>2</sub> _Au <sub>7</sub>	-1154.55	-7.6965	-4.1345	3.562	9.58702	1.781	-5.9155	4.912
NO <sub>2</sub> _Au <sub>8</sub>	-1290.17	-7.0233	-3.1201	3.9032	6.44968	1.9516	-5.0717	3.295
NO <sub>2</sub> _Au <sub>9</sub>	-1425.84	-6.7008	-4.0765	2.6243	23.86492	1.3121	-5.3887	5.5326
NO <sub>2</sub> _Au <sub>10</sub>	-1561.5	-6.0026	-3.1511	2.8515	19.7258	1.4257	-4.5768	3.6731
NO <sub>2</sub> _Au <sub>11</sub>	-1697.15	-6.7909	-4.1076	2.6833	20.76948	1.3417	-5.4492	5.5331
NO <sub>2</sub> _Au <sub>12</sub>	-1832.81	-6.3286	-3.1671	3.1614	10.1824	1.5807	-4.7478	3.5652
NO <sub>2</sub> _Au <sub>13</sub>	-1968.49	-6.6385	-4.1269	2.5116	28.87001	1.2558	-5.3827	5.7679
NO <sub>2</sub> _Au <sub>14</sub>	-2104.14	-6.3041	-2.9886	3.3154	11.81274	1.6577	-4.6463	3.2558
NO <sub>2</sub> _Au <sub>15</sub>	-2239.83	-6.4973	-3.3171	3.1802	5.89019	1.5901	-4.9072	3.786
NO <sub>2</sub> _Au <sub>16</sub>	-2375.47	-5.8953	-3.2218	2.6735	9.29601	1.3368	-4.5586	3.8864
NO <sub>2</sub> _Au <sub>17</sub>	-2511.15	-6.3541	-3.2537	3.1005	5.97422	1.5502	-4.8039	3.7216
NO <sub>2</sub> _Au <sub>18</sub>	-2646.81	-5.7451	-3.064	2.6811	15.44672	1.3406	-4.4046	3.6179
NO <sub>2</sub> _Au <sub>19</sub>	-2782.49	-6.7335	-3.4501	3.2833	0.36416	1.6417	-5.0918	3.9482
NO <sub>2</sub> _Au <sub>20</sub>	-2918.15	-6.3163	-2.5168	3.7995	15.37673	1.8998	-4.4165	2.5669
NO	-129.807	-8.6472	-2.1848	6.4624	-	3.2312	-5.416	2.2695
NO_Au <sub>1</sub>	-265.416	-7.4029	-3.329	4.0738	45.43311	2.0369	-5.366	3.534
NO_Au <sub>2</sub>	-401.074	-7.4725	-2.8588	4.6137	4.94468	2.3068	-5.1657	2.8918
NO_Au <sub>3</sub>	-536.699	-6.7759	-3.07	3.7059	29.95048	1.853	-4.9229	3.2698
NO_Au <sub>4</sub>	-672.367	-6.4589	-2.965	3.4939	4.21153	1.747	-4.7119	3.1772

<b>NO_Au5</b>	-808.012	-6.6741	-3.6537	3.0205	26.68333	1.5102	-5.1639	4.4142
<b>NO_Au6</b>	-943.694	-7.4034	-2.316	5.0874	0.64836	2.5437	-4.8597	2.3211
<b>NO_Au7</b>	-1079.33	-6.2151	-3.8754	2.3396	40.61477	1.1698	-5.0453	5.4399
<b>NO_Au8</b>	-1215.01	-7.0018	-2.753	4.2488	1.83352	2.1244	-4.8774	2.7995
<b>NO_Au9</b>	-1350.64	-6.4415	-2.7179	3.7236	8.0275	1.8618	-4.5797	2.8163
<b>NO_Au10</b>	-1486.3	-6.4861	-3.0626	3.4235	3.62311	1.7117	-4.7744	3.3292
<b>NO_Au11</b>	-1621.97	-6.7199	-3.1788	3.541	4.55606	1.7705	-4.9493	3.4589
<b>NO_Au12</b>	-1757.64	-6.5024	-3.1304	3.372	4.1991	1.686	-4.8164	3.4397
<b>NO_Au13</b>	-1893.28	-6.3356	-3.258	3.0776	12.84056	1.5388	-4.7968	3.7382
<b>NO_Au14</b>	-2028.96	-6.5302	-2.7832	3.747	0.33249	1.8735	-4.6567	2.8936
<b>NO_Au15</b>	-2164.6	-6.1571	-3.1892	2.9679	1.1787	1.484	-4.6731	3.679
<b>NO_Au16</b>	-2300.28	-6.1715	-3.1149	3.0567	3.70483	1.5283	-4.6432	3.5266
<b>NO_Au17</b>	-2435.94	-6.0271	-3.7021	2.3249	29.49507	1.1625	-4.8646	5.0892
<b>NO_Au18</b>	-2571.62	-6.3296	-3.1818	3.1478	0.7285	1.5739	-4.7557	3.5925
<b>NO_Au19</b>	-2707.24	-5.3598	-3.7671	1.5927	51.66753	0.7963	-4.5635	6.5378
<b>NO_Au20</b>	-2843	-6.9253	-2.5669	4.3584	2.9288	2.1792	-4.7461	2.5841
<b>SO2</b>	-548.358	-11.1371	-4.4371	6.7	-	3.35	-7.7871	4.5253
<b>SO2_Au1</b>	-684.017	-8.0423	-2.3873	5.6551	24.25225	2.8275	-5.2148	2.4044
<b>SO2_Au2</b>	-819.65	-7.1356	-3.5807	3.5549	26.75897	1.7774	-5.3582	4.0381
<b>SO2_Au3</b>	-955.351	-8.0652	-2.7715	5.2937	0.06238	2.6469	-5.4183	2.7729
<b>SO2_Au4</b>	-1090.98	-7.3019	-3.63	3.6719	9.52068	1.836	-5.466	4.0683
<b>SO2_Au5</b>	-1226.68	-7.8295	-3.4613	4.3682	6.02942	2.1841	-5.6454	3.648
<b>SO2_Au6</b>	-1362.26	-7.4026	-3.6716	3.731	27.13744	1.8655	-5.5371	4.1088
<b>SO2_Au7</b>	-1497.97	-7.1046	-3.8183	3.2863	16.58502	1.6432	-5.4615	4.5381
<b>SO2_Au8</b>	-1633.57	-7.0197	-3.8412	3.1786	23.8166	1.5893	-5.4304	4.6388
<b>SO2_Au9</b>	-1769.3	-6.8897	-2.6874	4.2023	21.91534	2.1011	-4.7885	2.7283
<b>SO2_Au10</b>	-1904.97	-7.2752	-2.8705	4.4047	23.99921	2.2024	-5.0729	2.9212
<b>SO2_Au11</b>	-2040.6	-6.2613	-3.9195	2.3418	30.85304	1.1709	-5.0904	5.5326
<b>SO2_Au12</b>	-2176.28	-6.672	-3.415	3.2569	7.46917	1.6285	-5.0435	3.905
<b>SO2_Au13</b>	-2311.93	-6.5852	-2.9478	3.6373	3.01048	1.8187	-4.7665	3.1231
<b>SO2_Au14</b>	-2447.6	-6.5876	-4.2349	2.3527	37.41987	1.1763	-5.4113	6.223
<b>SO2_Au15</b>	-2583.26	-5.6194	-2.8961	2.7233	9.32308	1.3617	-4.2578	3.3284
<b>SO2_Au16</b>	-2718.93	-6.4276	-2.9064	3.5212	19.46395	1.7606	-4.667	3.0929
<b>SO2_Au17</b>	-2854.59	-6.1979	-3.319	2.879	12.69143	1.4395	-4.7585	3.9325

<b>SO<sub>2</sub>_Au<sub>18</sub></b>	-2990.25	-6.3106	-3.5173	2.7932	11.91144	1.3966	-4.914	4.3224
<b>SO<sub>2</sub>_Au<sub>19</sub></b>	-3125.93	-6.636	-3.5916	3.0444	7.61387	1.5222	-5.1138	4.295
<b>SO<sub>2</sub>_Au<sub>20</sub></b>	-3261.56	-6.8543	-3.9791	2.8752	35.96294	1.4376	-5.4167	5.1024

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**Table S16**

The obtained values of natural charge and natural electron configuration for surface adsorption of CH<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, NO, NO<sub>2</sub>, and SO<sub>2</sub> gases with Ag<sub>16</sub> metallic silver cluster. NBO calculations were done using M06-2X/SDD method

System	Atom	Atom label	Natural Charge	Natural Electron Configuration
<b>CH<sub>4</sub></b>	C	1	-0.874	[core]2S(1.16)2p(3.72)
	H	2	0.2185	1S(0.78)
	H	3	0.2185	1S(0.78)
	H	4	0.2185	1S(0.78)
	H	5	0.2185	1S(0.78)
<b>CO</b>	C	1	0.51449	[core]2S(1.69)2p(1.76)3S(0.03)3p(0.01)
	O	2	-0.51449	[core]2S(1.76)2p(4.74)3S(0.01)
<b>CO<sub>2</sub></b>	C	1	1.07149	[core]2S(0.69)2p(2.22)3p(0.01)
	O	2	-0.53575	[core]2S(1.76)2p(4.76)3p(0.01)
	O	3	-0.53575	[core]2S(1.76)2p(4.76)3p(0.01)
<b>H<sub>2</sub>O</b>	O	1	-0.97859	[core]2S( 1.76)2p( 5.21)3p( 0.01)
	H	2	0.4893	1S( 0.51)
	H	3	0.4893	1S( 0.51)
<b>NO</b>	N	1	0.20809	[core]2S(1.75)2p(3.01)3S(0.02)3p(0.02)
	O	2	-0.20809	[core]2S(1.78)2p(4.42)3S(0.01)3p(0.01)
<b>NO<sub>2</sub></b>	N	1	0.53737	[core]2S( 1.28)2p( 3.14)3S( 0.02)3p( 0.02)
	O	2	-0.26869	[core]2S( 1.80)2p( 4.46)3p( 0.01)
	O	3	-0.26869	[core]2S( 1.80)2p( 4.46)3p( 0.01)
<b>SO<sub>2</sub></b>	S	1	1.37913	[core]3S(1.70)3p(2.87)4S(0.03)4p(0.02)
	O	2	-0.68957	[core]2S(1.90)2p(4.78)
	O	3	-0.68957	[core]2S(1.90)2p(4.78)
<b>Ag<sub>16</sub></b>	Ag	1	0.12583	[core]5S(0.76)4d(9.99)5p(0.13)
	Ag	2	0.13507	[core]5S(0.60)4d(9.99)5p(0.28)
	Ag	3	-0.36463	[core]5S(0.55)4d(9.99)5p(0.81)6d(0.02)
	Ag	4	-0.33304	[core]5S(0.62)4d(9.99)5p(0.72)6d(0.02)
	Ag	5	0.12219	[core]5S(0.65)4d(9.99)5p(0.24)
	Ag	6	0.077	[core]5S(0.68)4d(9.99)5p(0.25)
	Ag	7	-0.36463	[core]5S(0.55)4d(9.99)5p(0.81)6d(0.02)

	Ag	8	0.13507	[core]5S(0.60)4d(9.99)5p(0.28)
	Ag	9	-0.33304	[core]5S(0.62)4d(9.99)5p(0.72)6d(0.02)
	Ag	10	0.077	[core]5S(0.68)4d(9.99)5p(0.25)
	Ag	11	0.20783	[core]5S(0.65)4d(9.99)5p(0.15)
	Ag	12	-0.02718	[core]5S(0.77)4d(9.99)5p(0.26)6p(0.01)
	Ag	13	0.23011	[core]5S(0.69)4d(9.99)5p(0.09)6p(0.01)
	Ag	14	0.17448	[core]5S(0.62)4d(9.99)5p(0.22)
	Ag	15	0.01574	[core]5S(0.71)4d(9.99)5p(0.29)
	Ag	16	0.12219	[core]5S(0.65)4d(9.99)5p(0.24)
<b>CH<sub>4</sub>/Ag<sub>16</sub></b>	Ag	1	0.12286	[core]5S(0.75)4d(9.99)5p(0.14)
	Ag	2	0.13767	[core]5S(0.60)4d(9.99)5p(0.28)
	Ag	3	-0.36833	[core]5S(0.54)4d(9.99)5p(0.83)6d(0.02)
	Ag	4	-0.3268	[core]5S(0.62)4d(9.99)5p(0.71)6d(0.02)
	Ag	5	0.12891	[core]5S(0.65)4d(9.99)5p(0.24)
	Ag	6	0.08875	[core]5S(0.68)4d(9.99)5p(0.25)
	Ag	7	-0.35127	[core]5S(0.54)4d(9.99)5p(0.81)6d(0.02)
	Ag	8	0.13792	[core]5S(0.60)4d(9.99)5p(0.28)
	Ag	9	-0.33266	[core]5S(0.62)4d(9.99)5p(0.72)6d(0.02)
	Ag	10	0.08609	[core]5S(0.68)4d(9.99)5p(0.25)
	Ag	11	0.14694	[core]5S(0.63)4d(9.99)5p(0.23)7p(0.01)
	Ag	12	-0.02998	[core]5S(0.77)4d(9.99)5p(0.26)6p(0.01)
	Ag	13	0.21547	[core]5S(0.70)4d(9.99)5p(0.09)7p(0.01)
	Ag	14	0.17427	[core]5S(0.62)4d(9.99)5p(0.23)
	Ag	15	0.01688	[core]5S(0.71)4d(9.99)5p(0.29)
	Ag	16	0.12623	[core]5S(0.65)4d(9.99)5p(0.24)
		C	17	-0.87191
	H	18	0.23677	1S(0.76)
	H	19	0.21874	1S(0.78)
	H	20	0.22234	1S(0.78)
	H	21	0.22112	1S(0.78)
<b>CO/Ag<sub>16</sub></b>	Ag	1	0.11395	[core]5S(0.77)4d(9.99)5p(0.13)
	Ag	2	0.13533	[core]5S(0.60)4d(9.99)5p(0.28)
	Ag	3	-0.35152	[core]5S(0.55)4d(9.99)5p(0.80)6d(0.02)
	Ag	4	-0.35085	[core]5S(0.62)4d(9.99)5p(0.73)6d(0.02)
	Ag	5	0.06504	[core]5S(0.58)4d(9.99)5p(0.37)
	Ag	6	0.06976	[core]5S(0.69)4d(9.99)5p(0.25)
	Ag	7	-0.36826	[core]5S(0.55)4d(9.99)5p(0.82)6d(0.02)
	Ag	8	0.13063	[core]5S(0.59)4d(9.99)5p(0.30)
	Ag	9	-0.30717	[core]5S(0.63)4d(9.99)5p(0.68)6d(0.01)
	Ag	10	0.0748	[core]5S(0.69)4d(9.99)5p(0.26)

	Ag	11	0.20717	[core]5S(0.66)4d(9.99)5p(0.15)
	Ag	12	-0.02884	[core]5S(0.78)4d(9.99)5p(0.26)6p(0.01)
	Ag	13	0.22245	[core]5S(0.70)4d(9.99)5p(0.09)7p(0.01)
	Ag	14	0.16861	[core]5S(0.63)4d(9.99)5p(0.22)
	Ag	15	0.01527	[core]5S(0.71)4d(9.99)5p(0.29)
	Ag	16	0.11851	[core]5S(0.66)4d(9.99)5p(0.24)
	C	17	0.60539	[core]2S(1.65)2p(1.72)3S(0.02)3p(0.01)
	O	18	-0.52028	[core]2S(1.74)2p(4.77)3S(0.01)
<b>CO<sub>2</sub>/Ag<sub>16</sub></b>	Ag	1	0.09613	[core]5S(0.76)4d(9.99)5p(0.15)
	Ag	2	0.14438	[core]5S(0.60)4d(9.99)5p(0.27)
	Ag	3	-0.439	[core]5S(0.56)4d(9.99)5p(0.88)6d(0.02)
	Ag	4	-0.29063	[core]5S(0.60)4d(9.99)5p(0.69)6d(0.01)
	Ag	5	0.13938	[core]5S(0.65)4d(9.99)5p(0.23)
	Ag	6	0.08856	[core]5S(0.68)4d(9.99)5p(0.25)
	Ag	7	-0.36795	[core]5S(0.50)4d(9.99)5p(0.87)6d(0.02)
	Ag	8	0.13945	[core]5S(0.60)4d(9.99)5p(0.27)7p(0.01)
	Ag	9	-0.37726	[core]5S(0.62)4d(9.99)5p(0.76)6d(0.02)
	Ag	10	0.08927	[core]5S(0.67)4d(9.99)5p(0.26)
	Ag	11	0.20934	[core]5S(0.65)4d(9.99)5p(0.16)
	Ag	12	-0.02831	[core]5S(0.78)4d(9.99)5p(0.26)6p(0.01)
	Ag	13	0.23652	[core]5S(0.69)4d(9.99)5p(0.09)7p(0.01)
	Ag	14	0.17729	[core]5S(0.62)4d(9.99)5p(0.22)
	Ag	15	0.01733	[core]5S(0.70)4d(9.99)5p(0.30)
	Ag	16	0.09464	[core]5S(0.66)4d(9.99)5p(0.26)
	C	17	1.11169	[core]2S(0.68)2p(2.19)3p(0.02)
	O	18	-0.50023	[core]2S(1.75)2p(4.74)3p(0.01)
	O	19	-0.54059	[core]2S(1.73)2p(4.80)3p(0.01)
<b>H<sub>2</sub>O/Ag<sub>16</sub></b>	Ag	1	0.12953	[core]5S( 0.75)4d( 9.99)5p( 0.14)
	Ag	2	0.13812	[core]5S( 0.60)4d( 9.99)5p( 0.28)
	Ag	3	-0.40652	[core]5S( 0.53)4d( 9.99)5p( 0.88)6d( 0.02)
	Ag	4	-0.34654	[core]5S( 0.63)4d( 9.99)5p( 0.72)6d( 0.02)
	Ag	5	0.1243	[core]5S( 0.67)4d( 9.99)5p( 0.23)
	Ag	6	0.08197	[core]5S( 0.72)4d( 9.99)5p( 0.22)
	Ag	7	-0.35544	[core]5S( 0.61)4d( 9.99)5p( 0.74)6p( 0.01)6d( 0.02)
	Ag	8	0.20058	[core]5S( 0.49)4d( 9.98)5p( 0.32)6p( 0.01)
	Ag	9	-0.26866	[core]5S( 0.54)4d( 9.99)5p( 0.73)6d( 0.01)
	Ag	10	0.03154	[core]5S( 0.68)4d( 9.99)5p( 0.30)
	Ag	11	0.20321	[core]5S( 0.65)4d( 9.99)5p( 0.16)
	Ag	12	-0.01817	[core]5S( 0.76)4d( 9.99)5p( 0.27)6p( 0.01)
	Ag	13	0.19971	[core]5S( 0.72)4d( 9.99)5p( 0.10)



	Ag	14	0.16478	[core]5S( 0.63)4d( 9.99)5p( 0.22)
	Ag	15	-0.04041	[core]5S( 0.73)4d( 9.99)5p( 0.32)
	Ag	16	0.09034	[core]5S( 0.65)4d( 9.99)5p( 0.27)
	O	17	-1.01039	[core]2S( 1.73)2p( 5.27)3p( 0.01)
	H	18	0.53872	1S( 0.46)
	H	19	0.54334	1S( 0.46)
<b>NO/Ag<sub>16</sub></b>	Ag	1	0.18087	[core]5S(0.63)4d(9.99)5p(0.21)
	Ag	2	0.34496	[core]5S(0.44)4d(9.96)5p(0.26)6p(0.01)
	Ag	3	-0.36528	[core]5S(0.65)4d(9.99)5p(0.71)5d(0.02)
	Ag	4	0.07278	[core]5S(0.44)4d(9.97)5p(0.52)5d(0.01)6p(0.01)
	Ag	5	0.08502	[core]5S(0.70)4d(9.99)5p(0.23)6p(0.01)
	Ag	6	0.0373	[core]5S(0.69)4d(9.99)5p(0.28)6p(0.01)
	Ag	7	-0.27213	[core]5S(0.55)4d(9.99)5p(0.73)5d(0.01)
	Ag	8	0.14306	[core]5S(0.60)4d(9.99)5p(0.27)6p(0.01)
	Ag	9	-0.46384	[core]5S(0.63)4d(9.99)5p(0.83)5d(0.02)
	Ag	10	0.03461	[core]5S(0.79)4d(9.99)5p(0.20)
	Ag	11	0.14311	[core]5S(0.69)4d(9.99)5p(0.18)6p(0.01)
	Ag	12	0.05574	[core]5S(0.67)4d(9.99)5p(0.29)
	Ag	13	0.30585	[core]5S(0.62)4d(9.99)5p(0.08)6p(0.01)
	Ag	14	0.11952	[core]5S(0.65)4d(9.99)5p(0.25)
	Ag	15	0.16658	[core]5S(0.49)4d(9.97)5p(0.38)
	Ag	16	0.09914	[core]5S(0.74)4d(9.99)5p(0.18)
	N	17	-0.43566	[core]2S(1.62)2p(3.78)3S(0.01)3p(0.03)
	O	18	-0.25162	[core]2S(1.74)2p(4.49)3p(0.02)
<b>NO<sub>2</sub>/Ag<sub>16</sub></b>	Ag	1	0.23276	[core]5S(0.73)4d(9.99)5p(0.05)
	Ag	2	0.42674	[core]5S(0.39)4d(9.99)5p(0.20)6p(0.01)
	Ag	3	-0.01629	[core]5S(0.39)4d(9.98)5p(0.65)6S(0.01)5d(0.01)
	Ag	4	-0.37438	[core]5S(0.39)4d(9.98)5p(0.99)6S(0.01)5d(0.02)
	Ag	5	0.39166	[core]5S(0.39)4d(9.97)5p(0.26)
	Ag	6	0.18403	[core]5S(0.55)4d(9.99)5p(0.28)
	Ag	7	-1.77436	[core]5S(0.63)4d(9.98)5p(2.12)6S(0.01)5d(0.03)
	Ag	8	0.37629	[core]5S(0.52)4d(9.99)5p(0.12)
	Ag	9	-0.01885	[core]5S(0.50)4d(9.99)5p(0.53)5d(0.01)
	Ag	10	0.30363	[core]5S(0.60)4d(9.99)5p(0.11)
	Ag	11	0.25549	[core]5S(0.50)4d(9.99)5p(0.26)
	Ag	12	0.21656	[core]5S(0.57)4d(9.99)5p(0.24)
	Ag	13	0.25863	[core]5S(0.70)4d(9.99)5p(0.06)
	Ag	14	0.31373	[core]5S(0.59)4d(9.99)5p(0.12)
	Ag	15	0.04709	[core]5S(0.52)4d(9.99)5p(0.46)
	Ag	16	-0.19592	[core]5S(0.50)4d(9.98)5p(0.70)5d(0.01)

	N	17	0.48114	[core]2S(1.49)2p(3.00)3S(0.01)3p(0.02)
	O	18	-0.63514	[core]2S(1.76)2p(4.87)3p(0.01)
	O	19	-0.47281	[core]2S(1.76)2p(4.70)3p(0.01)
<b>SO<sub>2</sub>/Ag<sub>16</sub></b>	Ag	1	0.58285	[core]5S(0.32)4d(9.96)5p(0.15)
	Ag	2	0.12448	[core]5S(0.48)4d(9.99)5p(0.42)
	Ag	3	-0.25985	[core]5S(0.57)4d(9.99)5p(0.69)6d(0.02)
	Ag	4	-0.43277	[core]5S(0.57)4d(9.99)5p(0.87)6d(0.01)
	Ag	5	0.42641	[core]5S(0.01)4d(9.96)5p(0.36)7S(0.26)
	Ag	6	0.16456	[core]5S(0.69)4d(9.99)5p(0.16)
	Ag	7	-0.54308	[core]5S(0.57)4d(9.98)5p(0.98)6d(0.02)
	Ag	8	-0.4898	[core]5S(0.55)4d(9.99)5p(0.93)7S(0.01)6d(0.02)
	Ag	9	-0.14768	[core]5S(0.53)4d(9.98)5p(0.62)6d(0.01)7p(0.01)
	Ag	10	0.22695	[core]5S(0.67)4d(9.99)5p(0.12)
	Ag	11	0.18175	[core]5S(0.74)4d(9.99)5p(0.09)
	Ag	12	0.26254	[core]5S(0.66)4d(9.99)5p(0.09)
	Ag	13	0.2096	[core]5S(0.74)4d(9.99)5p(0.06)
	Ag	14	0.49501	[core]5S(0.37)4d(9.96)5p(0.19)
	Ag	15	0.11815	[core]5S(0.71)4d(9.99)5p(0.19)
	Ag	16	0.57161	[core]5S(0.30)4d(9.96)5p(0.17)
		S	17	0.73293
	O	18	-1.09662	[core]2S(1.86)2p(5.23)3p(0.01)
	O	19	-1.12705	[core]2S(1.85)2p(5.27)3p(0.01)

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