

Electronic Supplementary Information

C_3 -symmetry Mo_3S_4 aminophosphino Clusters Combining Three Sources of Stereogenicity: Stereocontrol directed by Hydrogen Bond Interactions and Ligand Configuration

Carmina Alfonso,^a Marta Feliz,^b Vicent S. Safont,^a and Rosa Llusar.^{,a}*

^a Departament de Química Física i Analítica, Universitat Jaume I, Av. Sos Baynat s/n, 12071 Castelló, Spain.

^b Instituto de Tecnología Química, CSIC-UPV, Avda. de los Naranjos, s/n, 46022, Valencia, Spain.

Table S1. Optimized energies (in a.u.) and Cartesian atomic coordinates (in Å) of the computed structures

(P)-[Mo-(S_N,R_C)]⁺

E = -2451.18813071 a.u.

Mo	1.37043500	-0.86824300	-0.83290600
P	3.14219200	-2.25847800	0.58280200
C	4.97946400	-1.84550400	0.65683200
C	2.49677100	-1.66492700	3.28595500
H	2.46788300	-0.63068300	2.95296400
C	5.90455000	-2.84220700	1.04129100
H	5.57448300	-3.85220000	1.27489400
C	2.76380100	-2.70458400	2.36955100
C	2.26362700	-1.95991300	4.64103900
H	2.06651600	-1.15088700	5.33978500
C	7.72306400	-1.22486200	0.89284400
H	8.77981400	-0.98580500	0.98087900
C	2.28758100	-3.29443800	5.09127700
H	2.10869200	-3.52167600	6.13916900
C	2.78900400	-4.04014600	2.82277200
H	2.99232000	-4.86078600	2.14008900
C	5.43224000	-0.53661800	0.40078300
H	4.73234000	0.23165000	0.09196300
C	2.54804500	-4.33324800	4.17856200
H	2.56923400	-5.36566300	4.51804600
C	6.80104200	-0.22940300	0.52145200
H	7.14388000	0.78197200	0.31866500
C	7.27139700	-2.53387900	1.15310800
H	7.97613600	-3.30671800	1.44903300
S	0.00608900	0.00362300	-2.65607600
S	-0.08695900	-2.07194000	0.61133000
Cl	3.36342300	-0.18361200	-2.26790000
N	1.60799700	-2.75393000	-2.11010000
H	0.79092900	-3.29701900	-1.78985500
C	1.52558700	-2.73336700	-3.62820700
H	2.16134600	-1.91837600	-3.97863000
H	0.49286400	-2.54596700	-3.92218100
C	2.05149900	-4.12732300	-4.09094000
H	1.23148700	-4.76253900	-4.44099500
H	2.75672600	-4.01146100	-4.92050700
C	3.04026100	-3.89653500	-0.37418400
H	3.94381000	-4.49532300	-0.22422100
H	2.17967300	-4.46312200	0.00107700
C	2.87244500	-3.56329400	-1.85713300
H	3.69549600	-2.91673900	-2.18413300
C	2.74510400	-4.74962500	-2.83721600
H	3.72337000	-5.18167000	-3.07196800
H	2.12689900	-5.54383300	-2.39745600
Mo	-1.43465300	-0.75374100	-0.84137200
P	-3.52633000	-1.59196400	0.57349300

C	-4.10841500	-3.38274500	0.64771500
C	-2.70784800	-1.43145900	3.28599300
H	-1.83647300	-1.98979700	2.95359300
C	-5.43074800	-3.66362100	1.05969200
H	-6.11879300	-2.86044800	1.31469000
C	-3.70816900	-1.05154500	2.36518200
C	-2.83060500	-1.08994600	4.64433200
H	-2.05815600	-1.39455100	5.34602300
C	-4.98682900	-6.05450800	0.88553900
H	-5.32522100	-7.08369000	0.97451700
C	-3.94916900	-0.36103300	5.09432200
H	-4.04498400	-0.09919200	6.14504800
C	-4.82768100	-0.32290800	2.81782800
H	-5.61405100	-0.01823400	2.13278600
C	-3.22604300	-4.44364200	0.36665900
H	-2.21392400	-4.23796000	0.03786100
C	-4.94528500	0.02309500	4.17773800
H	-5.81211700	0.58453200	4.51701100
C	-3.66693600	-5.77570500	0.48736700
H	-2.98208700	-6.58964700	0.26426100
C	-5.86929200	-4.99412700	1.17234400
H	-6.88792800	-5.20135400	1.48978700
S	-1.74760700	1.10015500	0.61600500
Cl	-1.83532400	-2.81338000	-2.29255900
N	-3.18218800	-0.00591800	-2.11247200
H	-3.23851900	0.97161400	-1.78618000
C	-3.12368100	0.06446300	-3.63056300
H	-2.73083500	-0.88910900	-3.98727600
H	-2.44854900	0.87028300	-3.91873700
C	-4.59462100	0.30225800	-4.09389800
H	-4.73562000	1.32697000	-4.45221000
H	-4.84752000	-0.37357800	-4.91745800
C	-4.88953500	-0.67247200	-0.37742600
H	-5.86202000	-1.15055000	-0.22450200
H	-4.94334000	0.35660700	-0.00271800
C	-4.51877100	-0.69104400	-1.86142100
H	-4.37713900	-1.72621500	-2.19470000
C	-5.47939400	0.02176000	-2.83783200
H	-6.34986800	-0.60042200	-3.07020400
H	-5.84685500	0.95807800	-2.39646900
Mo	0.06909600	1.61805100	-0.83143900
P	0.37992100	3.84517600	0.59094800
C	-0.88833100	5.23819900	0.64921400
C	0.13820600	3.00724600	3.29527500
H	-0.75090200	2.48334000	2.95407900
C	-0.48092500	6.53703500	1.02812200
H	0.55889500	6.75019200	1.26623000
C	0.93204700	3.73692500	2.38459800
C	0.49278500	2.95122900	4.65492800
H	-0.13014600	2.39258300	5.34892300
C	-2.78426200	7.31897200	0.86146500
H	-3.51440900	8.12038900	0.94051600
C	1.64570400	3.61675900	5.11573100
H	1.91833800	3.57474500	6.16720100
C	2.08592900	4.40321600	2.84822800
H	2.71653400	4.97186600	2.17010400

C	-2.24858600	4.98409700	0.38728400
H	-2.56907100	3.99443600	0.08256600
C	2.44237700	4.33986700	4.20870600
H	3.33349000	4.85650900	4.55620400
C	-3.19229600	6.02350800	0.49549600
H	-4.23971000	5.82102400	0.28747200
C	-1.42455500	7.57402400	1.12810300
H	-1.10230400	8.57015000	1.42003700
S	1.82699200	0.95487200	0.62735400
Cl	-1.50750400	3.00539000	-2.27654600
N	1.59728200	2.76519900	-2.09181700
H	2.47082200	2.32296100	-1.76514700
C	1.63382400	2.68776000	-3.61007600
H	0.61415200	2.83748300	-3.96900000
H	1.98487700	1.69853800	-3.90397700
C	2.58831800	3.83619800	-4.06097000
H	3.54926700	3.43961900	-4.40389900
H	2.14527000	4.39408500	-4.89246400
C	1.86347300	4.57035100	-0.34756000
H	1.93435900	5.65132700	-0.19321800
H	2.77842800	4.10234100	0.03514500
C	1.67150700	4.26365200	-1.83379100
H	0.70542500	4.65940000	-2.16960700
C	2.77439600	4.74307400	-2.80271600
H	2.66841900	5.80763900	-3.03559900
H	3.76632800	4.59709000	-2.35416600

(P)-[Mo-(S_N,S_C)]⁺

E = -2451.19680402 a.u.

H	1.94741700	2.38003100	-2.06311800
H	-0.51561300	5.19387400	-1.58025100
H	0.53214900	5.96882000	-0.38560300
H	-5.51193000	6.56050500	1.75777800
H	-0.88934100	2.75588100	3.13765100
H	-5.57309100	4.36800700	0.56211100
H	1.91155900	5.49623000	1.27702700
H	2.30143500	4.51553800	5.45393400
H	0.30020700	3.02352300	5.29467600
H	-3.31221400	7.56338200	2.39565200
H	3.09444600	5.74140100	3.42686900
H	2.24281700	4.13337300	-0.70995200
H	-3.45874000	3.20089700	-0.01853500
H	-1.20311900	6.38287200	1.86251000
H	1.47820100	6.08890600	-2.78439100
H	3.09893500	5.46575100	-2.46286300
H	2.88800900	3.73809100	-4.10602500
H	1.69098000	4.83566400	-4.81375600
H	-0.16007400	3.67602600	-3.65207500
H	0.88946600	2.32004200	-4.10222300
C	0.25654200	5.00455500	-0.82675600
C	0.42013000	4.10540700	2.04617000
C	-2.18396300	4.70856800	0.87249600

C	-4.58640200	6.04552900	1.51289600
C	-0.02120900	3.40886500	3.19313200
C	-4.62001500	4.81024800	0.84074400
C	1.54879000	4.94408500	2.13970000
C	1.78069600	4.39892400	4.50698600
C	0.65325400	3.55831200	4.41670300
C	-3.34730800	6.61227500	1.87076800
C	2.22673900	5.08945700	3.36592700
C	1.47975000	4.32802500	-1.47156800
C	-3.42338900	4.14155500	0.51805400
C	-2.15041700	5.94529300	1.55698400
C	2.06253600	5.17035500	-2.65588200
C	1.94521400	4.26480400	-3.91490100
C	0.84132700	3.25665100	-3.54389000
N	1.09754100	2.97335300	-2.07290200
P	-0.54927900	3.87038100	0.45382800
S	1.57668000	1.30188500	0.63497500
S	0.00265600	-0.00392300	-2.66258600
Cl	-2.11538200	2.61359400	-2.28877700
Mo	-0.25518500	1.59720600	-0.83381300
H	-3.02211700	0.49979200	-2.07247400
H	-4.27943700	-3.02262900	-1.56548300
H	-5.45319700	-2.47533400	-0.36241600
H	-2.97887700	-8.05342300	1.73905600
H	-1.94895300	-2.21469000	3.14948500
H	-1.04065600	-7.02114600	0.54857800
H	-5.68442700	-1.01948900	1.29447800
H	-5.01590400	-0.26901200	5.48351400
H	-2.75321800	-1.32184400	5.31520700
H	-4.93908900	-6.63835200	2.37584200
H	-6.46622900	-0.12426800	3.45439900
H	-4.68108100	-0.09234300	-0.70045900
H	-1.07095100	-4.60377800	-0.02792500
H	-4.95254800	-4.21899000	1.84955300
H	-6.03981300	-1.71495500	-2.75464700
H	-6.26700000	0.00950700	-2.45053500
H	-4.67020800	0.63361000	-4.11667900
H	-5.04949900	-0.95703900	-4.79753300
H	-3.12400200	-1.98944000	-3.63584900
H	-2.45864400	-0.41604800	-4.10626800
C	-4.47955800	-2.25216400	-0.81281300
C	-3.75630900	-1.68847500	2.05987600
C	-3.01066800	-4.24313600	0.86357000
C	-2.98793000	-6.99376900	1.49647400
C	-2.93576500	-1.76067300	3.20764900
C	-1.89611900	-6.41133200	0.82759200
C	-5.02911000	-1.09160700	2.15823100
C	-4.66461200	-0.66025800	4.53220900
C	-3.38979600	-1.25334300	4.43680900
C	-4.09376600	-6.19741700	1.85401300
C	-5.48119000	-0.57946500	3.39012900
C	-4.48622400	-0.85616300	-1.46140200
C	-1.90536600	-5.03975100	0.50815200
C	-4.10416700	-4.82653100	1.54390100
C	-5.51249200	-0.76080800	-2.64004900
C	-4.66994300	-0.44310100	-3.90855800

C	-3.24939500	-0.90994100	-3.53878000
N	-3.12103500	-0.53211300	-2.07213900
P	-3.08615700	-2.40536700	0.45705600
S	-1.91627300	0.71300200	0.63434000
Cl	-1.20997400	-3.14006900	-2.28951900
Mo	-1.25675400	-1.02345000	-0.83426300
H	1.08260400	-2.86858800	-2.07688500
H	4.76166800	-2.19442700	-1.56048400
H	4.87133500	-3.48144000	-0.35316300
H	8.46980200	1.45232400	1.72962000
H	2.92413200	-0.56898400	3.15350100
H	6.56973800	2.63739100	0.62276800
H	3.71675100	-4.40899500	1.29796100
H	2.75210600	-4.19498000	5.49131700
H	2.55235300	-1.70728400	5.32285800
H	8.26023100	-0.97581900	2.28747000
H	3.33263000	-5.52928000	3.46087000
H	2.42206500	-4.00322000	-0.69225900
H	4.49005600	1.40418400	0.05090100
H	6.17208000	-2.19792700	1.76627900
H	4.50851900	-4.38889600	-2.73535400
H	3.11313800	-5.43104300	-2.44442400
H	1.80942100	-4.35583200	-4.13054100
H	3.38529900	-3.88345700	-4.78618300
H	3.29771600	-1.70578300	-3.62319600
H	1.60604800	-1.91708000	-4.10468100
C	4.19317600	-2.75045700	-0.80713300
C	3.34934700	-2.40164500	2.06410700
C	5.18427500	-0.48032300	0.86012500
C	7.55623200	0.91458800	1.48880400
C	3.01445700	-1.65127300	3.21299800
C	6.48533500	1.58152200	0.86671700
C	3.45952400	-3.80310600	2.16259300
C	2.91488800	-3.69686800	4.53902500
C	2.80201400	-2.29542000	4.44350600
C	7.43971500	-0.45409600	1.80179800
C	3.24262500	-4.44791500	3.39604300
C	2.98691000	-3.45567900	-1.45488400
C	5.30150200	0.88780800	0.54933700
C	6.25708800	-1.14853500	1.49413400
C	3.41741000	-4.39600100	-2.63073900
C	2.73797200	-3.81740700	-3.90577500
C	2.42596300	-2.35543300	-3.53285200
N	2.02501900	-2.43702700	-2.06973000
P	3.62951700	-1.46529200	0.45910700
S	0.33950700	-2.02148400	0.63277700
Cl	3.32661400	0.52570100	-2.27964400
Mo	1.51366600	-0.57975800	-0.83272000

$(M)-[\text{Mo}-(S_N, R_C)]^+$

E = -2451.16325534 a.u.

Mo	-1.59728400	-0.40354300	-0.93725000
P	-3.75206000	-1.00722900	0.51686900
C	-3.57479100	-1.59584400	2.29991300
C	-5.20595400	1.06668500	1.79630600
H	-4.42981800	1.00868200	2.55435600
C	-4.54642700	-2.44931400	2.86697500
H	-5.39543100	-2.79421600	2.28177100
C	-5.18453200	0.20445500	0.67784500
C	-6.24095300	2.00525700	1.95023200
H	-6.24555300	2.66122800	2.81711700
C	-3.38446200	-2.38056800	5.01044200
H	-3.31030100	-2.68460000	6.05141200
C	-7.26836200	2.08932100	0.99139300
H	-8.07304500	2.80984200	1.11349100
C	-6.20396900	0.30600900	-0.29113700
H	-6.19586500	-0.31002300	-1.18467600
C	-2.51782700	-1.12469600	3.10477000
H	-1.77364400	-0.45320000	2.68623400
C	-7.24596600	1.23722100	-0.12783300
H	-8.02911100	1.30058900	-0.87892000
C	-2.42454500	-1.51547800	4.45417600
H	-1.60568100	-1.14689600	5.06715900
C	-4.44823900	-2.84481900	4.21281600
H	-5.20242500	-3.50243500	4.63704200
S	-0.01904000	-0.01717700	-2.78382500
S	-1.43694100	1.51078100	0.46105900
Cl	-3.44023100	0.88220700	-2.24624800
N	-2.69981700	-1.98483300	-2.18434900
H	-3.45360000	-1.35389900	-2.49099000
C	-2.15233200	-2.62686700	-3.46164700
H	-1.06673100	-2.63686500	-3.43484700
H	-2.48655300	-2.01578500	-4.30637700
C	-2.72589500	-4.07087000	-3.49781600
H	-3.09169600	-4.33812400	-4.49416300
H	-1.93858300	-4.78243900	-3.22571600
C	-4.42412700	-2.51244900	-0.44428100
H	-4.76544500	-3.27502300	0.26092600
H	-5.28966300	-2.19119100	-1.03354500
C	-3.34589800	-3.09803100	-1.36868400
H	-2.55225700	-3.57271100	-0.78283700
C	-3.85469100	-4.08866200	-2.43734700
H	-4.02628000	-5.08766700	-2.02311600
H	-4.80332100	-3.73164600	-2.86395600
Mo	0.44502700	1.56346500	-0.95671200
P	1.03297500	3.74261200	0.48085000
C	0.40326100	3.90667900	2.25032100
C	3.50697700	4.08976300	1.84887400
H	3.03036300	3.54650200	2.65948300
C	0.13434700	5.18002200	2.79824700
H	0.26957100	6.08146800	2.20580700
C	2.80111700	4.36884100	0.65756400

C	4.83435000	4.52643200	2.00654600
H	5.36455200	4.30761800	2.92983700
C	-0.42915500	4.16129300	4.94149500
H	-0.75260800	4.25920200	5.97460600
C	5.46970800	5.24855800	0.97899400
H	6.49357900	5.59165400	1.10367000
C	3.44799700	5.07645700	-0.37769400
H	2.95070800	5.26619400	-1.32290900
C	0.27114200	2.76433800	3.06590600
H	0.49518100	1.78066000	2.66381900
C	4.77203900	5.52139700	-0.21219600
H	5.25669000	6.06928100	-1.01596500
C	-0.14304000	2.89236300	4.40536800
H	-0.24254900	2.00544800	5.02629700
C	-0.28592800	5.30643000	4.13431500
H	-0.49047200	6.29226300	4.54343900
S	2.01978700	0.48283000	0.45645900
Cl	2.47414100	2.48195400	-2.29902100
N	-0.37235300	3.30740100	-2.21009800
H	0.54752400	3.62711400	-2.54394900
C	-1.23657500	3.14658200	-3.46332000
H	-1.79992600	2.21983800	-3.41011900
H	-0.56277900	3.10825800	-4.32546600
C	-2.18464600	4.37797400	-3.49344300
H	-2.25644400	4.81200900	-4.49559500
H	-3.19065700	4.07058800	-3.18675900
C	0.10276700	5.08158300	-0.50853800
H	-0.35305200	5.80005700	0.17775700
H	0.83023000	5.62335600	-1.12315600
C	-0.97562900	4.44640800	-1.39748600
H	-1.77551200	4.01798200	-0.78524300
C	-1.59154400	5.37396400	-2.46585600
H	-2.34918800	6.04177900	-2.04266500
H	-0.80939700	5.99640300	-2.92414800
Mo	1.12494400	-1.18707300	-0.94353100
P	2.74185800	-2.74375100	0.51114000
C	3.18741800	-2.24160400	2.27281900
C	1.88209800	-5.06524800	1.92501900
H	1.65657600	-4.37899900	2.73586200
C	4.43867200	-2.59161100	2.82517000
H	5.17313900	-3.13942700	2.24019000
C	2.43732400	-4.59206900	0.71544400
C	1.62768900	-6.43717800	2.10079500
H	1.20318600	-6.78770600	3.03807700
C	3.80172800	-1.58989900	4.95624600
H	4.03951500	-1.33662200	5.98623700
C	1.92778000	-7.35093200	1.07328200
H	1.73777600	-8.41219000	1.21191300
C	2.71740000	-5.50895100	-0.32005500
H	3.09747000	-5.17231400	-1.27879800
C	2.23981700	-1.57937800	3.08024700
H	1.26566700	-1.32115000	2.67489100
C	2.47251300	-6.88182800	-0.13644900
H	2.69768400	-7.57758600	-0.94039600
C	2.54616600	-1.25658600	4.41580700
H	1.80812100	-0.74672600	5.03017400

C	4.74702600	-2.26134700	4.15716700
H	5.71465000	-2.53515400	4.56933400
S	-0.59435200	-1.99349300	0.48432800
Cl	0.89372400	-3.42287100	-2.24761300
N	3.03188700	-1.36899200	-2.21162900
H	2.85576300	-2.33670400	-2.51568900
C	3.30003100	-0.57348200	-3.49062500
H	2.78158400	0.37962500	-3.44620800
H	2.90958700	-1.15720600	-4.33043000
C	4.84039200	-0.37158800	-3.55810200
H	5.23350500	-0.56849600	-4.56036200
H	5.08302300	0.66477200	-3.29846400
C	4.36335300	-2.59962800	-0.48467600
H	5.21343400	-2.52632100	0.19884600
H	4.48633700	-3.51792300	-1.06960400
C	4.32992500	-1.37842200	-1.41492300
H	4.36204400	-0.45022800	-0.83539300
C	5.42642800	-1.34040900	-2.50040000
H	6.38695200	-0.99632100	-2.10271000
H	5.57577600	-2.34442300	-2.92351500

(M)-[Mo-(S_NS_C)]⁺

E = -2451.16396395 a.u.

H	3.05030000	-0.00337200	-2.89164900
H	5.42180600	-0.96189100	-0.04269800
H	5.52013600	-2.59646900	-0.70434100
H	4.78763400	-0.95610300	5.86411100
H	2.30491100	-4.06215000	2.40428900
H	2.46648200	-0.49375200	5.06506500
H	4.13721300	-4.34507300	-1.51555400
H	3.05089900	-7.92345000	0.62865600
H	2.17291400	-6.53050500	2.51141200
H	6.47168400	-1.92216900	4.28992200
H	4.03945900	-6.80766000	-1.37853300
H	4.19974100	-1.99494300	-2.66481400
H	1.83742000	-0.97450100	2.70732800
H	5.84596600	-2.43034100	1.95233800
H	6.68632400	-0.73980000	-2.22468900
H	5.78460800	-0.59246400	-3.73222900
H	5.31443000	1.65999800	-3.29371900
H	6.27232700	1.58281800	-1.81363300
H	4.35717500	1.04830200	-0.45703000
H	3.52226500	1.98256600	-1.70794600
C	4.87567000	-1.71543600	-0.61963200
C	3.24458700	-4.01951300	0.44272300
C	3.79648400	-1.71907100	2.15648000
C	4.51184300	-1.16894300	4.83440000
C	2.67735600	-4.65150400	1.57091800
C	3.20470000	-0.90904900	4.38360500
C	3.72737100	-4.80737200	-0.62341600
C	3.09960600	-6.83881500	0.57506300
C	2.60531800	-6.05460000	1.63498400

C	5.46236900	-1.71063000	3.94658500
C	3.66015200	-6.21098800	-0.55301000
C	4.53916100	-1.18122500	-2.02622400
C	2.84737500	-1.18157800	3.04871300
C	5.10546400	-1.98958500	2.61563600
C	5.73529600	-0.40563100	-2.65389400
C	5.45355400	1.10332800	-2.36015400
C	4.14954500	1.11293900	-1.52748400
N	3.41210500	-0.15103800	-1.93968600
P	3.31955100	-2.14104500	0.38568300
S	-0.01857900	-2.04437000	0.57809400
S	-0.00205400	-0.00393000	-2.69487000
Cl	1.80246700	-2.69804300	-2.55248500
Mo	1.41422200	-0.82837900	-0.87692100
H	-1.46253700	2.68394400	-2.91499500
H	-1.90019000	5.13040200	-0.01483600
H	-0.54129600	6.07954600	-0.62729400
H	-1.54303900	4.53012200	5.90076500
H	2.37745000	4.01059000	2.41089500
H	-0.78584900	2.30006500	5.06700100
H	1.67189900	5.74926100	-1.49931300
H	5.32792300	6.59944800	0.61928600
H	4.57847600	5.13573300	2.50417700
H	-1.55591800	6.49384100	4.35366800
H	3.85121400	6.89946000	-1.37553600
H	-0.33034400	4.67018000	-2.61735800
H	-0.06654100	2.02820200	2.70201600
H	-0.81333800	6.23834700	2.00900200
H	-2.67545700	6.18278700	-2.19569300
H	-2.30347500	5.37673100	-3.71857100
H	-4.02129100	3.82161900	-3.38051800
H	-4.48995500	4.65130100	-1.89547000
H	-3.11614800	3.22612900	-0.52266400
H	-3.45815900	2.07067900	-1.81964100
C	-0.96315400	5.07040200	-0.57842200
C	1.85276800	4.80738300	0.45554700
C	-0.40136600	4.10564600	2.18234400
C	-1.22489300	4.41236500	4.86803800
C	2.69299200	4.63120700	1.57675300
C	-0.79807700	3.15671100	4.39757500
C	2.28367200	5.62354500	-0.61178400
C	4.36508500	6.09709800	0.57194300
C	3.94318600	5.27315800	1.63292700
C	-1.23504100	5.51889300	3.99568000
C	3.53190100	6.26968100	-0.54921500
C	-1.22067900	4.54348100	-2.00326100
C	-0.38932300	3.00203700	3.05873800
C	-0.82038800	5.36783400	2.66087900
C	-2.47295400	5.20644000	-2.64976800
C	-3.64417700	4.19796600	-2.42281500
C	-3.02784200	3.04410100	-1.59662000
N	-1.54992000	3.04968100	-1.95719200
P	0.19091400	3.92892600	0.40620000
S	1.76458400	1.00232000	0.58715300
Cl	1.44824100	2.90335700	-2.55212800
Mo	0.00629400	1.64039200	-0.87883200

H	-1.61521300	-2.61541000	-2.90726500
H	-3.48407700	-4.20748200	0.01848500
H	-4.99388300	-3.52112000	-0.59340100
H	-3.17710300	-3.54118200	5.93098800
H	-4.70477300	0.04306200	2.41893600
H	-1.60406800	-1.79725600	5.07923300
H	-5.80242600	-1.42613500	-1.51023100
H	-8.41721500	1.27588500	0.59770000
H	-6.79372300	1.36688200	2.49810200
H	-4.88277900	-4.52922000	4.39361600
H	-7.90472700	-0.13767300	-1.39983200
H	-3.89200000	-2.63726200	-2.59297500
H	-1.72005400	-1.05944200	2.70876700
H	-5.02395800	-3.78017200	2.04190200
H	-4.01473600	-5.42659300	-2.14719900
H	-3.53797200	-4.70645000	-3.68402700
H	-1.31702400	-5.38767300	-3.38618600
H	-1.77084100	-6.22311600	-1.89960400
H	-1.22713300	-4.32200300	-0.52223500
H	-0.06696700	-4.03178800	-1.82769300
C	-3.90962100	-3.37453800	-0.55110500
C	-5.10471500	-0.80273500	0.45514700
C	-3.36537500	-2.37599200	2.19968800
C	-3.22984300	-3.21696100	4.89477500
C	-5.39116300	0.00467100	1.57765600
C	-2.34434900	-2.23489900	4.41418700
C	-6.01587200	-0.84124800	-0.62148200
C	-7.49454500	0.70261900	0.55628200
C	-6.58052400	0.75386000	1.62612200
C	-4.18955100	-3.77614000	4.02795500
C	-7.20821300	-0.09645900	-0.56643800
C	-3.33252700	-3.34165900	-1.97911000
C	-2.40988000	-1.81587900	3.07106900
C	-4.26061000	-3.35434500	2.68877500
C	-3.28411300	-4.76087100	-2.61977800
C	-1.81740700	-5.26050200	-2.41943800
C	-1.12291800	-4.15030100	-1.59618500
N	-1.87511400	-2.87584100	-1.94628800
P	-3.50575500	-1.79239300	0.41689100
S	-1.76951000	1.03404800	0.57166600
Cl	-3.23879700	-0.21178500	-2.56716200
Mo	-1.43118700	-0.81624300	-0.87834100