

Electronic Supporting Information

Influence of Halogen Bonding on Gold(I)-Ligand Bond Components

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Materials and Instrumentation. Unless otherwise noted, all reagents were purchased from commercial sources and used without further purification. ^1H and ^{13}C NMR spectra were recorded with a Bruker AVANCE DRX400 spectrometer equipped with a BBFO broadband probe. Chemical shifts were measured in ppm (δ) from TMS by residual solvent peaks for ^1H and ^{13}C . All the reactions involving gold have been conducted protecting the flask from light with an aluminum foil. The precursor $[(\text{NAC})\text{AuCl}]$ has been synthesized as described in literature.¹

Synthesis of 1BF_4 . $[(\text{NAC})\text{AuCl}]$ (100 mg, 0.259 mmol) and selenourea (32 mg, 0.259 mmol) were dissolved in dry dichloromethane, under Ar atmosphere, in a flask protected by light. AgBF_4 (55.5 g, 0.285 mmol) were added, causing the immediate formation of a grey-white solid (AgCl and the excess of AgBF_4). The mixture reaction was stirred for 30 minutes, then the solid was filtered off on a Celite pad and the volume of the solution was reduced to about 2 mL. Adding 5 mL of n-pentane caused the precipitation of a white solid with purple dots, which was filtered, washed with n-pentane (3 - 5 mL) and dried under vacuum. A small aliquot of the solid has been dissolved in 0.7 ml of CDCl_3 passed through activated alumina, in order to remove acid impurities and water. The NMR spectrum of the white portion (see Figure S1) confirms the initial formation of the desired product: the two triplets at 4.0 and 3.3 ppm are typical of the α protons of the pyrrolidine, together with the two multiplets around 2.0 ppm.² The singlet at 1.6 ppm is due to the tert-butyl group and the two broad signals 6.7 and 4.7 ppm are in agreement with a coordinated selenourea (if not coordinated, only one broad peak is present³). Anyway, the shape of the peaks underlines the presence of a second set of signals, likely due to the decomposition of the system. Indeed, the color of the solvent turned to purple, with the final formation of metallic gold in the tube and unidentified products in solution.

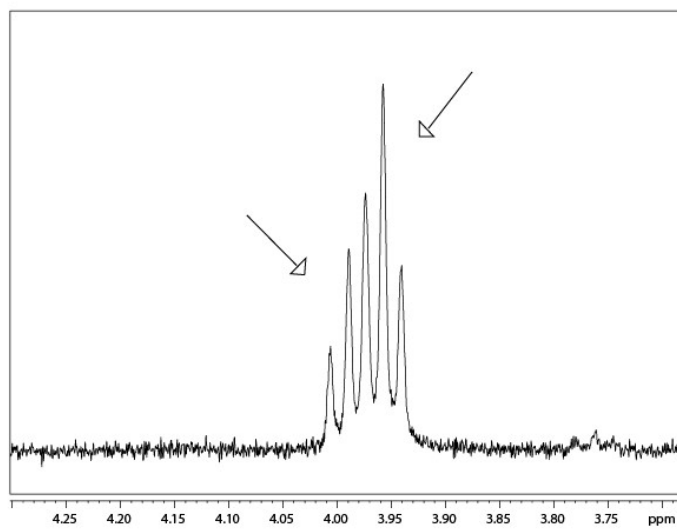
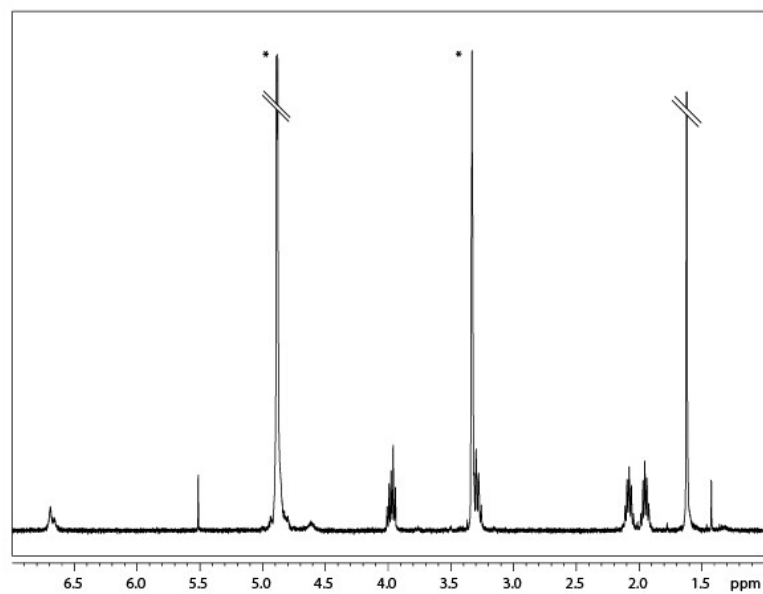


Figure S1. ¹H NMR spectrum of [(NAC)Au(SeU)]BF₄ in dry CDCl₃ (400 MHz, 23°C).

Table S1. Energy Decomposition Analysis results for the coordinative and noncovalent bonds.

Compound	Fragments	E_{int}	E_{oi}	E_{st}	E_{disp}
1	$[(\text{SeU})\text{Au}]^+ \cdots [\text{NAC}]$	-98.6	-78.8	-14.0	-9.9
	$[\text{SeU}] \cdots [\text{Au}(\text{NAC})]^+$	-66.1	-54.0	-6.2	-5.9
1-A1	$[(\text{SeU})(\text{A1})\text{Au}]^+ \cdots [\text{NAC}]$	-100.7	-75.9	-14.6	-10.2
	$[(\text{SeU})(\text{A1})] \cdots [\text{Au}(\text{NAC})]^+$	-62.1	-53.6	-1.3	-7.1
	$[\text{A1}] \cdots [(\text{SeU})\text{Au}(\text{NAC})]^+$	-4.4	-3.5	3.3	-4.1
1-A2	$[(\text{SeU})(\text{A2})\text{Au}]^+ \cdots [\text{NAC}]$	-101.3	-76.2	-14.6	-10.5
	$[(\text{SeU})(\text{A2})] \cdots [\text{Au}(\text{NAC})]^+$	-61.9	-53.5	-1.1	-7.3
	$[\text{A2}] \cdots [(\text{SeU})\text{Au}(\text{NAC})]^+$	-4.5	-3.8	3.6	-4.4
1-A3	$[(\text{SeU})(\text{A3})\text{Au}]^+ \cdots [\text{NAC}]$	-102.5	-79.8	-9.3	-13.4
	$[\text{SeU}] \cdots [\text{Au}(\text{A3})(\text{NAC})]^+$	-75.6	-63.0	-3.6	-9.0
	$[\text{A3}] \cdots [\text{Au}(\text{SeU})(\text{NAC})]^+$	-20.8	-16.7	5.5	-9.7
3	$[\text{ClAu}] \cdots [\text{NAC}]$	-85.7	-66.7	-10.1	-8.9
	$[\text{Cl}]^- \cdots [\text{Au}(\text{NAC})]^+$	-150.6	-65.0	-83.1	-2.4
3A3	$[(\text{A3})\text{ClAu}] \cdots [\text{NAC}]$	-92.6	-70.0	-13.3	-9.4
	$[(\text{A3})\text{Cl}]^- \cdots [\text{Au}(\text{NAC})]^+$	-126.7	-57.4	-64.9	-4.4
	$[\text{A3}] \cdots [\text{ClAu}(\text{NAC})]$	-13.4	-12.0	2.3	-3.7

Table S2. NOCV-CD analysis results.

Compound	Fragments	$\Delta\rho_0$	$\Delta\rho_1$	$\Delta\rho_2$	$\Delta\rho_3$	$\Delta\rho_{\text{tot,back}}$
1	$[(\text{SeU})\text{Au}]^+\cdots[\text{NAC}]$	0.359	-0.049	-0.030	-0.013	-0.092
	$[\text{SeU}]\cdots[\text{Au}(\text{NAC})]^+$	0.346	0.024	-0.021	-0.016	-0.037
1-A1	$[(\text{SeU})(\text{A1})\text{Au}]^+\cdots[\text{NAC}]$	0.364	-0.046	-0.030	-0.010	-0.086
	$[(\text{SeU})(\text{A1})]\cdots[\text{Au}(\text{NAC})]^+$	0.343	0.020	-0.021	-0.015	-0.036
	$[\text{A1}]\cdots[(\text{SeU})\text{Au}(\text{NAC})]^+$	-0.037	0.005	-	-	-
1-A2	$[(\text{SeU})(\text{A2})\text{Au}]^+\cdots[\text{NAC}]$	0.372	-0.040	-0.030	-0.010	-0.080
	$[(\text{SeU})(\text{A2})]\cdots[\text{Au}(\text{NAC})]^+$	0.344	0.020	-0.021	-0.015	-0.036
	$[\text{A2}]\cdots[(\text{SeU})\text{Au}(\text{NAC})]^+$	-0.039	0.005	-	-	-
1-A3	$[(\text{SeU})(\text{A3})\text{Au}]^+\cdots[\text{NAC}]$	0.375	-0.044	-0.027	-0.010	-0.081
	$[\text{SeU}]\cdots[\text{Au}(\text{A3})(\text{NAC})]^+$	0.373	0.033	-0.018	-0.014	-0.032
	$[\text{A3}]\cdots[\text{Au}(\text{SeU})(\text{NAC})]^+$	-0.106	0.024	-	-	-
3	$[\text{ClAu}]\cdots[\text{NAC}]$	0.321	-0.081	-0.039	-0.025	-0.145
	$[\text{Cl}]\cdots[\text{Au}(\text{NAC})]^+$	0.295	0.041	0.032	-0.013	-0.013
3A3	$[(\text{A3})\text{ClAu}]\cdots[\text{NAC}]$	0.337	-0.071	-0.038	-0.021	-0.130
	$[(\text{A3})\text{Cl}]\cdots[\text{Au}(\text{NAC})]^+$	0.275	0.025	0.024	0.003	-
	$[\text{A3}]\cdots[\text{ClAu}(\text{NAC})]$	-0.105	0.004	-	-	-

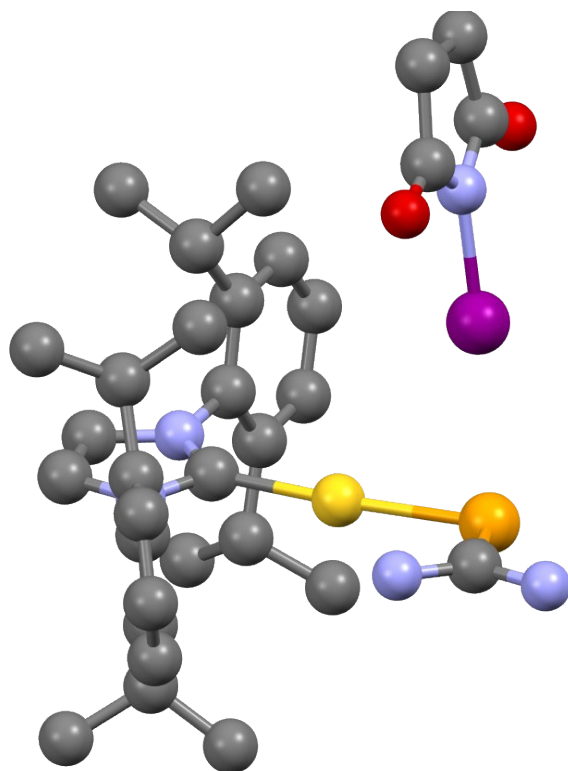


Figure S2. DFT-optimized geometry of **2A3**.

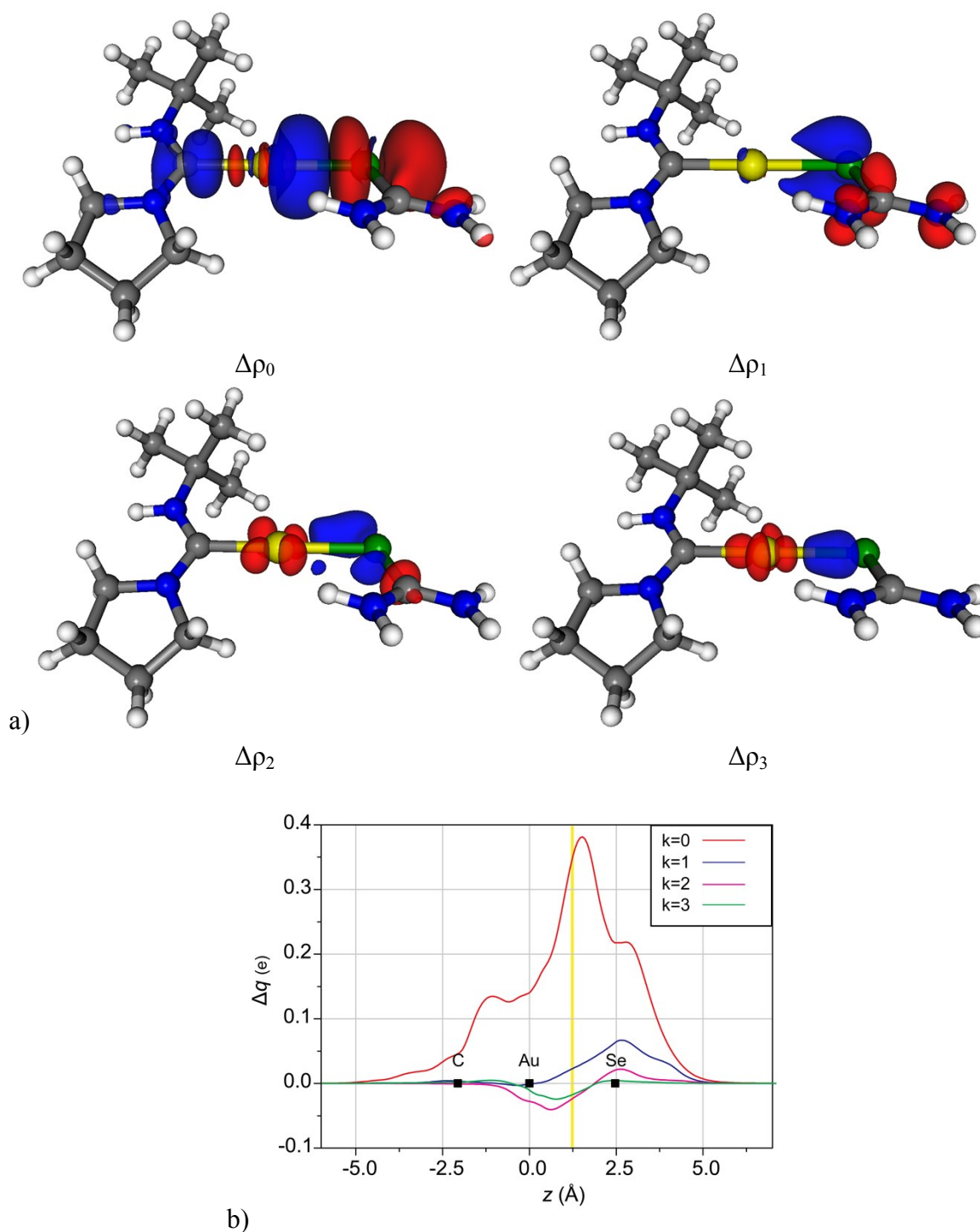


Figure S3. (a) Isodensity surfaces ($\pm 1.5 \text{ me/au}$) for the most relevant $\Delta\rho_k$ ($k = 0 - 3$) for the $[(\text{NAC})\text{Au}]^+ \cdots [\text{SeU}]$ bond in 1^+ . Blue and red regions indicate accumulation and depletion of electron density, respectively. (b) Most relevant CD_k curves for the $[(\text{NAC})\text{Au}]^+ \cdots [\text{SeU}]$ bond in 1^+ . Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

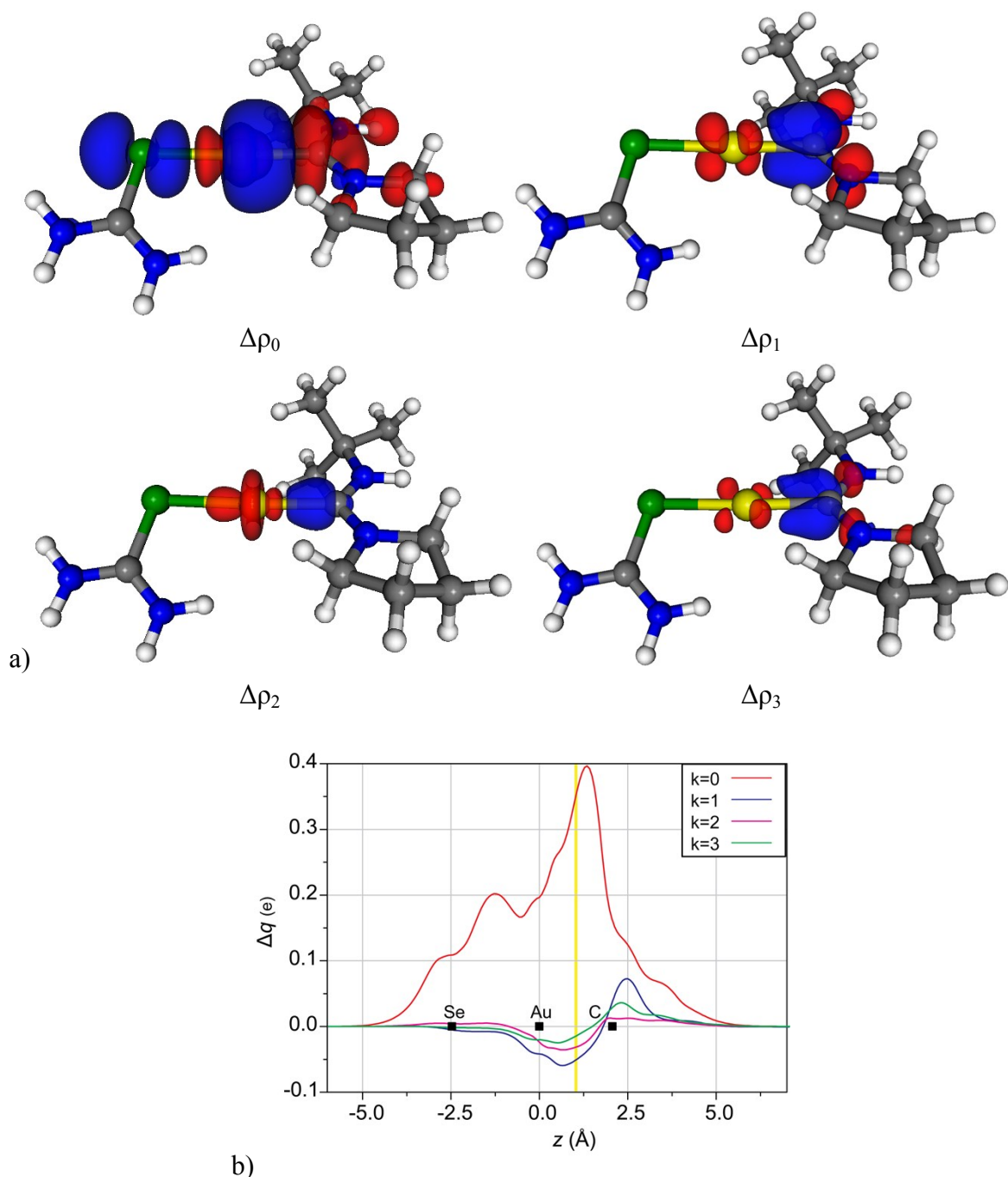


Figure S4. (a) Isodensity surfaces (± 1.5 me/au) for the most relevant $\Delta\rho_k$ ($k = 0 - 3$) for the $[(\text{SeU})\text{Au}]^+ \cdots [\text{NAC}]$ bond in $\mathbf{1}^+$. Blue and red regions indicate accumulation and depletion of electron density, respectively. (b) Most relevant CD_k curves for the $[(\text{SeU})\text{Au}]^+ \cdots [\text{NAC}]$ bond in $\mathbf{1}^+$. Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

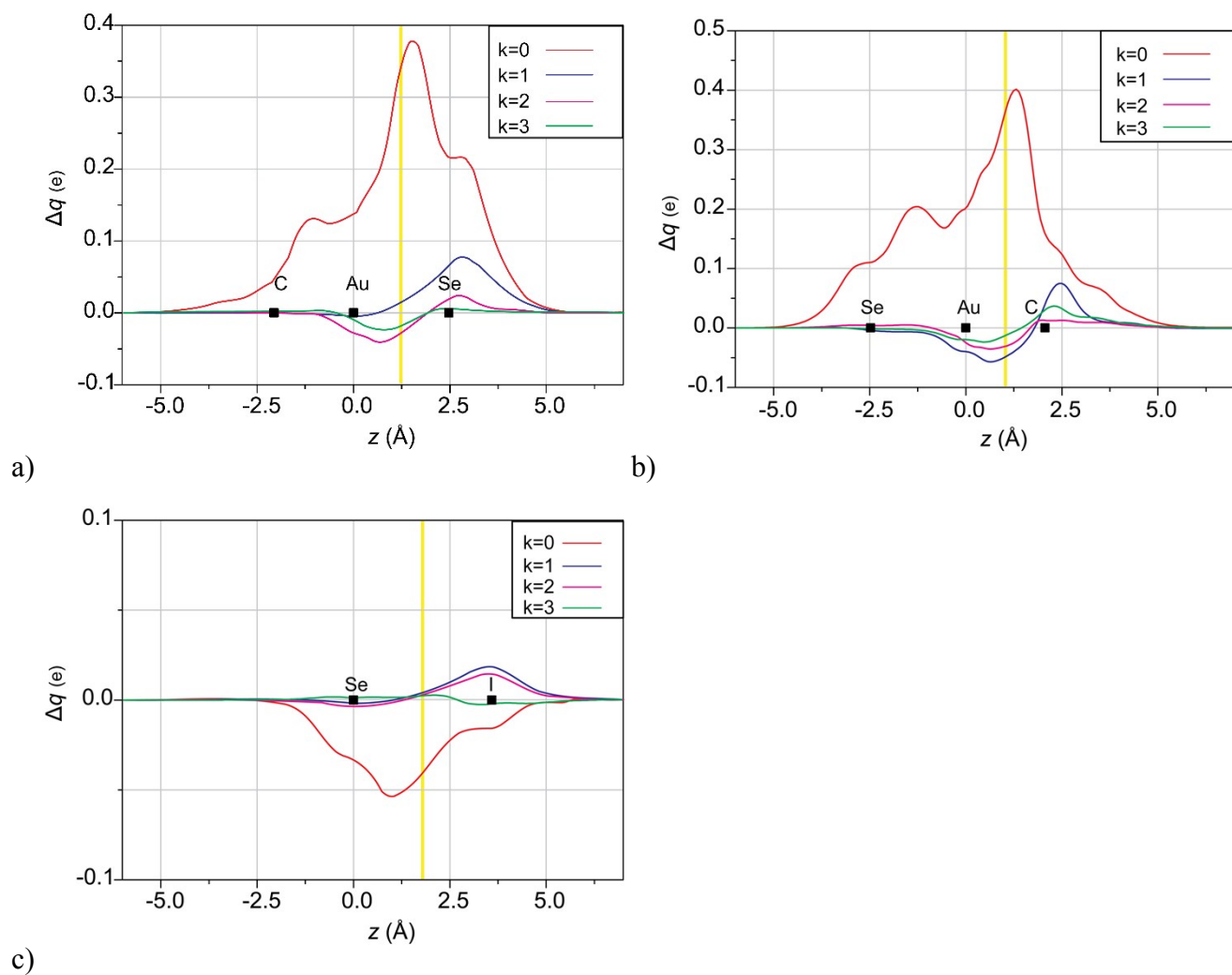


Figure S5. Most relevant CD_k curves for the a) $[(A1)(SeU)] \cdots [Au(NAC)]^+$ bond; b) $[(A1)(SeU)Au]^+ \cdots [NAC]$ bond; c) $[A1] \cdots [(SeU)Au(NAC)]^+$ bond in **1A1**. Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

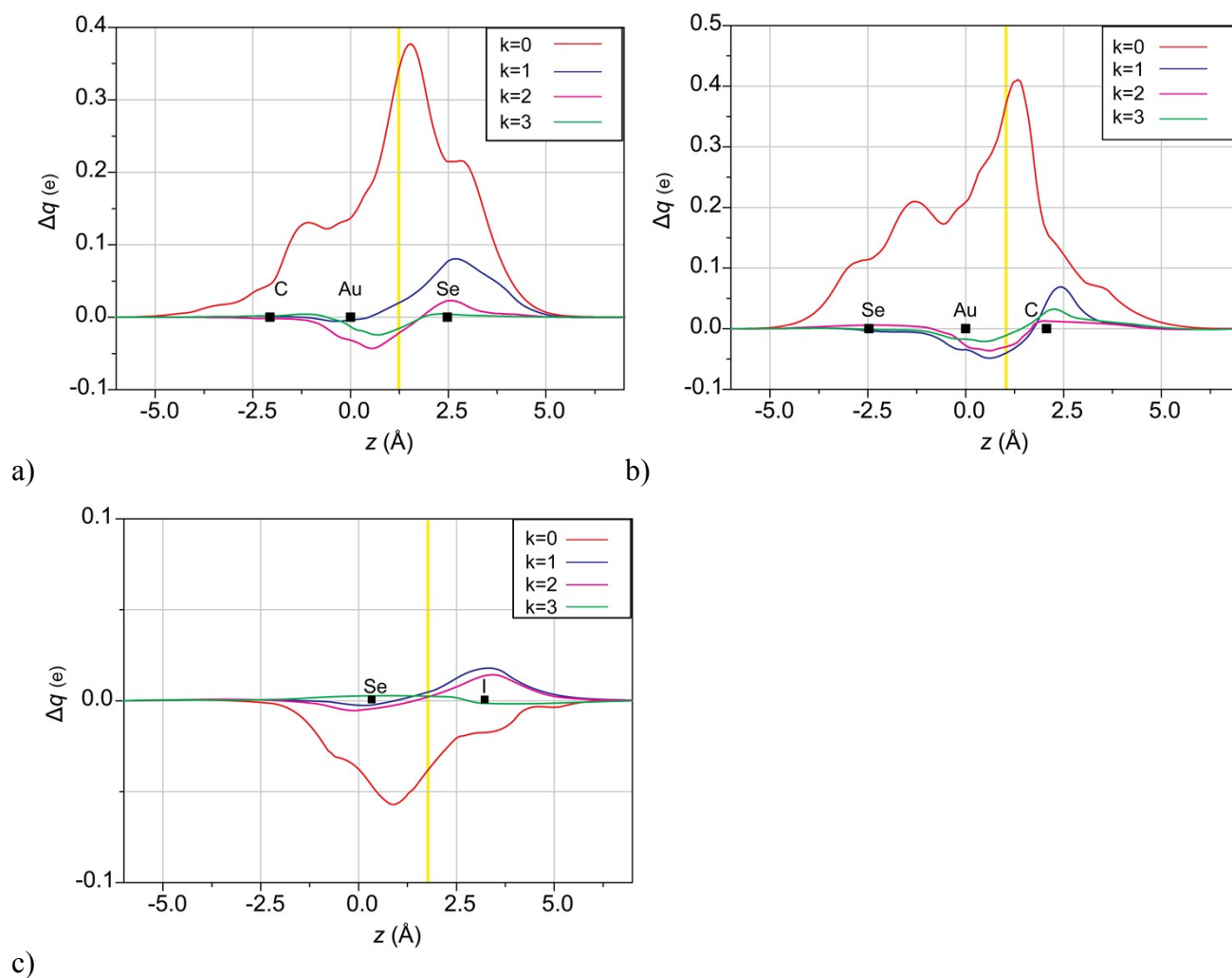


Figure S6. Most relevant CD_k curves for the a) $[(A2)(SeU)] \cdots [Au(NAC)]^+$ bond; b) $[(A2)(SeU)Au]^+ \cdots [NAC]$ bond; c) $[A2] \cdots [(SeU)Au(NAC)]^+$ bond in **1A2**. Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

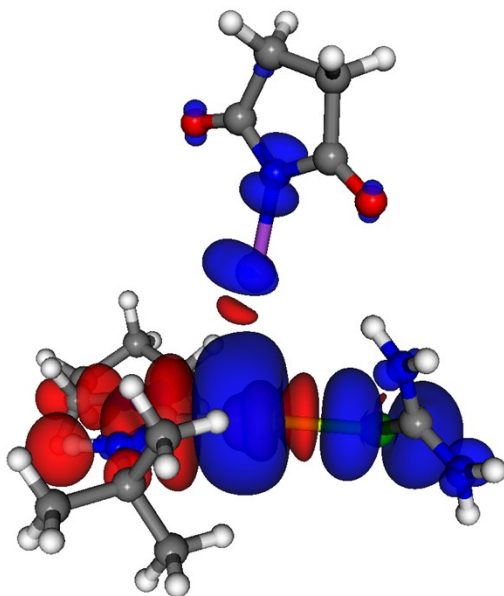


Figure S7. Isodensity surfaces (± 0.75 me/au) for the most relevant $\Delta\rho_k$ ($k = 0 - 3$) for the $[(\text{SeU})\text{Au}]^+\cdots[\text{NAC}]$ bond in $\mathbf{1}^+$. Blue and red regions indicate accumulation and depletion of electron density, respectively.

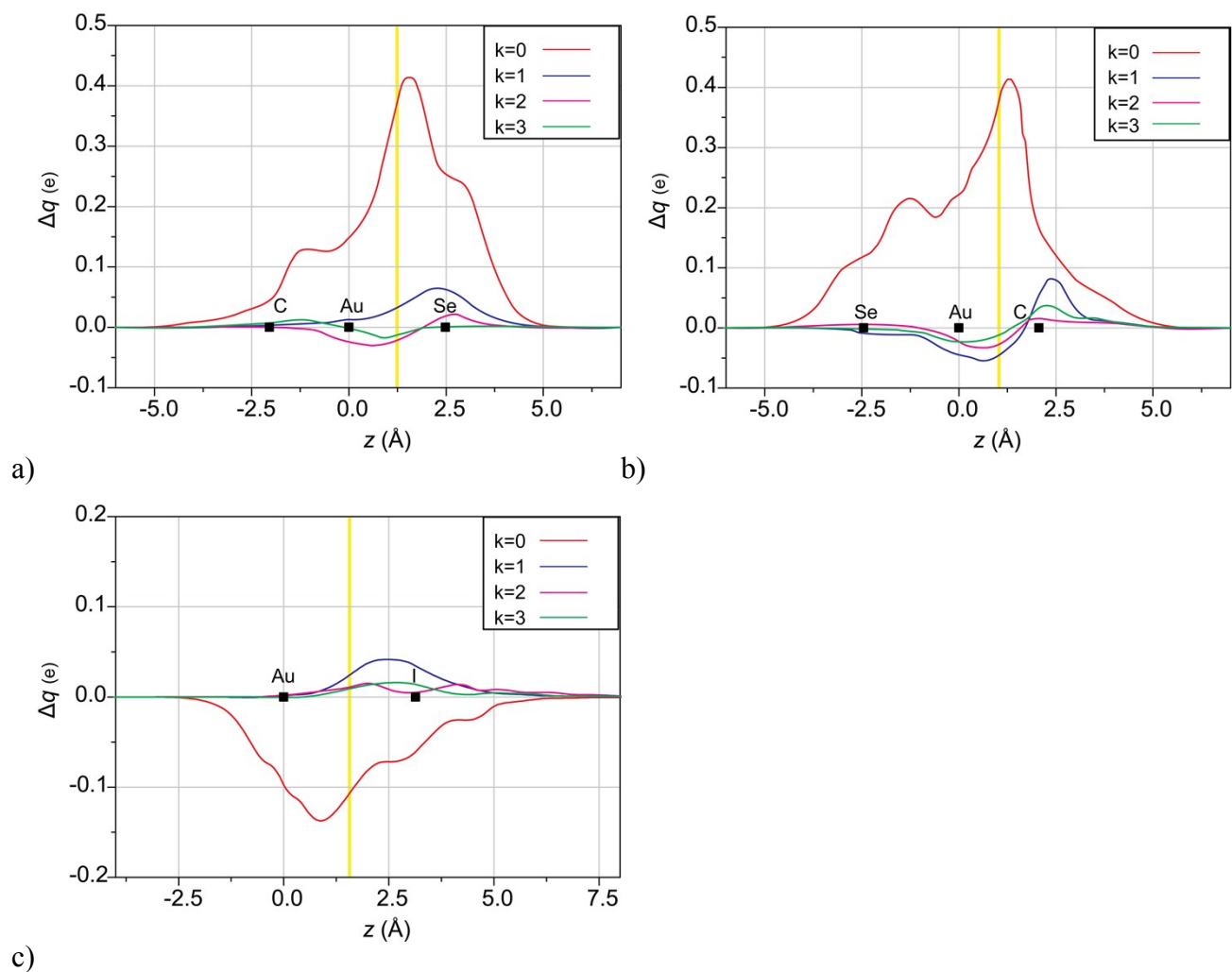


Figure S8. Most relevant CD_k curves for the a) $[(A3)(SeU)] \cdots [Au(NAC)]^+$ bond; b) $[(A3)(SeU)Au]^+ \cdots [NAC]$ bond; c) $[A3] \cdots [(SeU)Au(NAC)]^+$ bond in **1A3**. Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

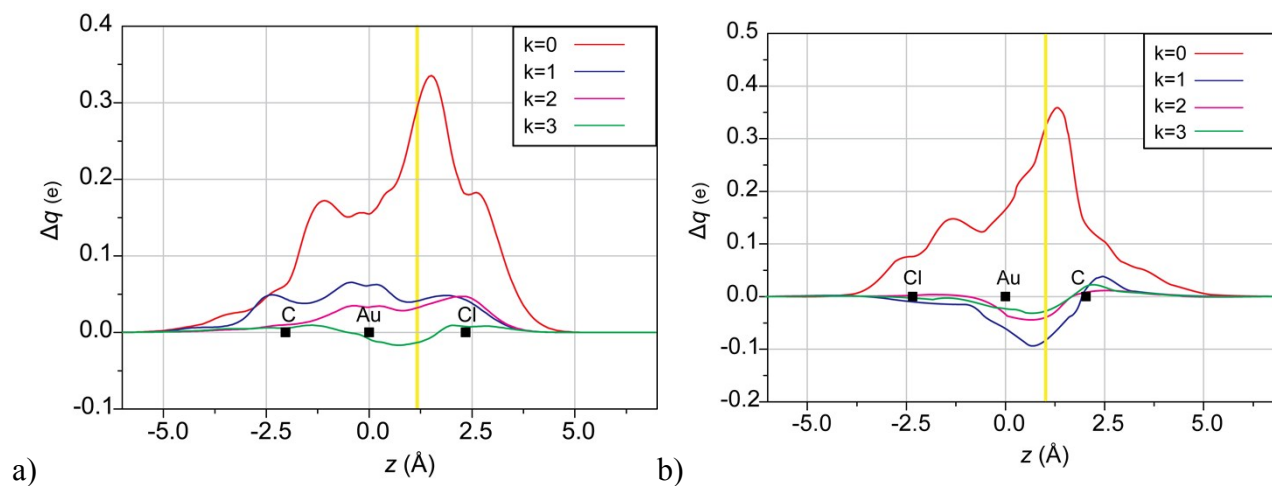


Figure S9. Most relevant CD_k curves for the a) [Cl]⁻...[Au(NAC)]⁺ bond; b) [ClAu]...[NAC] bond in **3**. Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

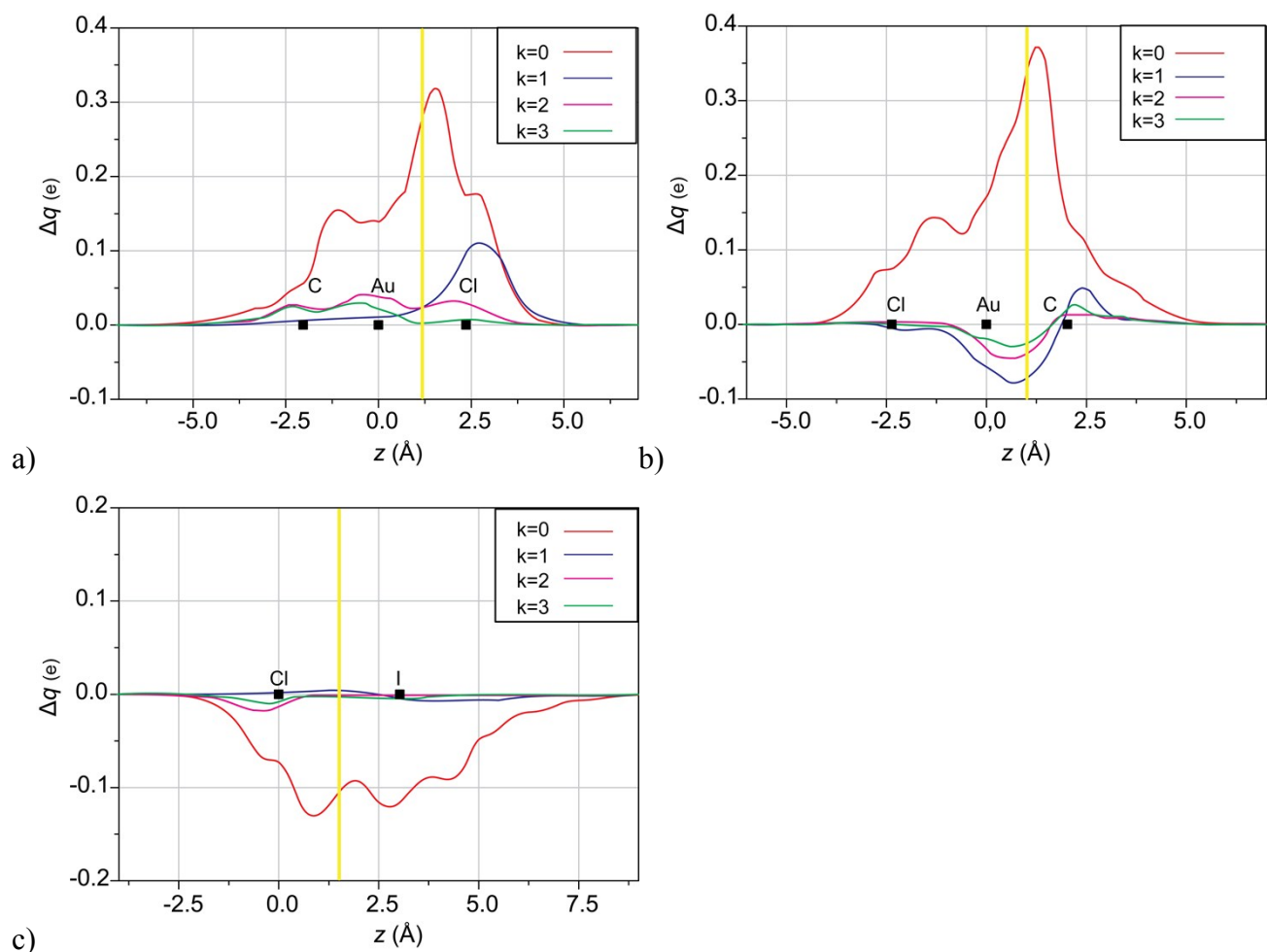


Figure S10. Most relevant CD_k curves for the a) [(A3)(Cl)]⁻⋯[Au(NAC)]⁺ bond; b) [(A3)(Cl)Au]⁻⋯[NAC] bond; c) [A3]⁻⋯[(Cl)Au(NAC)] bond in **3A3**. Black dots indicate the z position of the atomic nuclei. A yellow vertical band indicates the boundary between the fragments.

List of coordinates for all the optimized geometries

38

1+

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38

1+_TS

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43

1A1

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43

1A1TS

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C	0.63285928503253	2.67655909636335	2.76036216793116
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C	0.78092689033126	3.23414317509134	4.18076475823572
C	-0.49300950816054	3.40895321582041	2.02070403478016
H	-2.02546325710131	-2.91835625318584	3.89736534212847
H	-2.23600207970695	-3.53516729145531	2.26256220666713
H	0.06901891336794	-4.16050638153911	2.25352524792047
H	0.21134262590708	-3.52356199381303	3.88821459587368
H	0.74573233075979	-2.12381817687538	1.24948367587900
H	1.59593780776728	-1.90450364745784	2.79170346061249
H	-2.41067292553641	-0.81851385579807	2.80987762804930
H	-1.79937892736169	-1.43379513213254	1.26171465165713
H	1.56885576849305	2.71183595519231	4.72755605723223
H	-0.15477969277600	3.14370926336536	4.73699271441797
H	1.04479706635458	4.29035181531719	4.13085725939454
H	2.74964005621914	2.22903807979427	2.53161739405625
H	2.26243567976292	3.83245212539114	1.95920990210656
H	1.89013122215310	2.40209789971630	0.99234724856727
H	-0.62705756510376	3.02025368172916	1.01023280529612
H	-0.24316251760309	4.46827927210297	1.94711888690648
H	-1.43821160407839	3.31321063694759	2.55830863829815
H	0.16185802469353	0.92754438337696	3.90753034826266
Au	0.14993024338194	0.50211981214369	0.04166195968915
Se	0.38443941692332	0.81789666634680	-2.41168980393915
C	-0.44728188021418	-0.73108619395523	-3.15890304719527
N	-0.21075058622798	-0.99231788936870	-4.43227439122305
N	-1.24382471460473	-1.51674560279260	-2.45461806473164
H	-1.46193629840598	-1.28845680609796	-1.49763118729331

H	-1.68024294785986	-2.33541763659514	-2.85714217985470
H	0.42292695498139	-0.41623661289819	-4.96292521878866
H	-0.65346918672835	-1.76509008540346	-4.91124820520961
C	-3.82262622860824	4.73275292725942	-3.20242881174457
F	-3.28989115084112	5.94422937896736	-3.40560032326718
F	-4.58458899649370	4.43187945162100	-4.26135999425490
F	-4.61860190911424	4.80466236509089	-2.12754346516914
I	-2.25298107770623	3.22463100662545	-2.91191574975188

46

1A2

C	-3.19456361234137	-0.02195962291370	-3.25735383853120
C	-2.36368500413623	0.47179184110587	-4.44777470913014
C	-0.94503355930748	-0.00631119818507	-4.12302021442437
N	-0.91320908512580	-0.08158258411108	-2.64222165534516
C	-2.25352982883290	0.18353429033960	-2.07159294960358
C	0.16687665727609	-0.37077882263020	-1.92274789323232
N	1.29644113963051	-0.60942481581723	-2.59253674059192
C	2.65337403297571	-0.96942258406886	-2.07645092171438
C	3.21601924719411	0.15971309085158	-1.20340275425613
C	3.52932953552265	-1.13563478299930	-3.32501482593443
C	2.60505794639282	-2.29548932070988	-1.30601420128810
H	-3.42830982049037	-1.08294102019338	-3.36953911947654
H	-4.12981790660022	0.52311253743786	-3.13477346861425
H	-2.38671233526157	1.56262231866897	-4.49721010480586
H	-2.71056746273960	0.08287524360404	-5.40409695323864

H	-0.18065337715487	0.68289714441396	-4.48892513937879
H	-0.74647882703674	-0.99839667108321	-4.54054722007666
H	-2.44670043427536	-0.49235353638676	-1.24085578908575
H	-2.29940877821918	1.21409675133899	-1.70799710199703
H	3.57868344405258	-0.20554383028629	-3.89674074752351
H	3.14520260529956	-1.92788601228803	-3.97280778441811
H	4.54412429031678	-1.40335987629900	-3.03045393842748
H	3.25005198984355	1.09841200462847	-1.75995256101657
H	4.22949186822698	-0.09187299637009	-0.88625849071456
H	2.61004614382289	0.31029000314751	-0.30850966477523
H	1.98721635374328	-2.21743183483219	-0.40915198387336
H	3.61291067876098	-2.57527366991250	-0.99472589261372
H	2.20181162272138	-3.09303133173414	-1.93304150496815
H	1.25891272162207	-0.56226617071113	-3.60282760527830
Au	0.03240565813353	-0.43124415387711	0.13763018630824
Se	-0.11552771490366	-0.62146867758499	2.60442027915462
C	-1.30482935188610	0.78638309481592	3.10107993533624
N	-1.70103746117182	0.83569249388449	4.36270794730668
N	-1.72421115395320	1.69373200173666	2.23620987581439
H	-1.38206156532563	1.68020518154915	1.28804418066702
H	-2.35013686013680	2.44142487347543	2.50543579565133
H	-1.41182726819443	0.12910674489118	5.02073478262824
H	-2.29760334029931	1.57536367981348	4.70796429267241
C	4.64624284453562	1.84309943693802	4.69613851056161
C	5.69755146812952	2.26182467224011	3.62816974290808
I	2.85054449587595	0.92388767728173	3.81808826652368
F	4.30294073219095	2.94389111031530	5.39522796030962
F	5.23596457106264	0.97635174343518	5.54346724040430
F	5.17976956710173	3.16311352682287	2.78549712746895

F	6.10728509706003	1.19863573492399	2.92787565774647
F	6.76264003590075	2.80920631533378	4.23054399287237

46

1A2TS

C	-0.01766622656876	0.04332799381019	2.06853775871462
N	0.16211802528375	-1.17656720841469	2.77651359033003
C	-0.85173455062011	-2.21382095489796	2.46183653977813
C	-0.25859982024876	-3.48223822239987	3.09472563980894
C	1.27094889280005	-3.22938854022255	3.14389344915940
C	1.46342590977914	-1.84211737329145	2.51474286555661
N	-0.17360840282846	1.04865468648335	2.87324278972292
C	-0.39900237862444	2.50707995241215	2.59489164939559
C	0.78350589368229	3.07437963799247	1.80150266500386
C	-0.47928393488803	3.17876538585014	3.97057941383430
C	-1.72497334717735	2.68261779385738	1.84531788664086
H	-0.65566101764710	-3.62907204013194	4.09886730143358
H	-0.51753153225524	-4.36128517958189	2.50463177942123
H	1.83756647563194	-3.98218373275787	2.59622768313614
H	1.62627786301806	-3.23002882061170	4.17412469481764
H	1.64662597464286	-1.92585192033631	1.43394159238599
H	2.27719471244628	-1.26982483328919	2.95948734160521
H	-1.82023910393729	-1.93257002626192	2.87397338155045
H	-0.95903178718496	-2.33422820131067	1.37410955569259
H	0.45224907620601	3.04680390820290	4.52567826691614
H	-1.30289250468243	2.76901850104446	4.55981422840428
H	-0.65132831616979	4.24785863472220	3.84560883700959
H	1.72059542015287	2.92487444822948	2.34106133170615

H	0.63679137176495	4.14529125251906	1.65404478979809
H	0.87358568525993	2.60247493762164	0.82206038768388
H	-1.70788834486785	2.17089736667740	0.88178797293694
H	-1.90536783710047	3.74451030024304	1.67234552200706
H	-2.55649608349105	2.28034379761342	2.42652386362301
H	-0.14572066532823	0.79666972888004	3.86131269201591
Au	0.00823409367649	0.09010686429143	0.01961078408704
Se	0.16066915959267	-0.16105000988762	-2.44628559668020
C	-0.09412083199771	1.59364172372695	-3.15562244771619
N	0.17976978126910	1.77757733090399	-4.43610705952509
N	-0.53671650401212	2.59833885908446	-2.41956532825377
H	-0.80119982953502	2.44289092836119	-1.46078371222973
H	-0.68330386441394	3.52190030125769	-2.80527066386659
H	0.54857572815812	1.02503470456268	-4.99640024296071
H	0.03016528418731	2.66708634496653	-4.89313826322467
C	-5.03664894313761	-2.12196255172380	-4.00068472893701
C	-6.05575653893566	-2.27370101424342	-2.83428352067309
I	-3.07682804877930	-1.37979888973426	-3.33397879937071
F	-5.56348641747654	-1.27195129575731	-4.90534510869807
F	-4.89545464591393	-3.32580064348800	-4.58964893491454
F	-6.27271399176410	-1.09373634453260	-2.24223171444690
F	-5.60281456778443	-3.14057769888384	-1.92233705022734
F	-7.22337931018112	-2.72977988155538	-3.30930308245153

1A3

C	-3.44189945675108	-0.56720154833347	-3.28344096186978
C	-2.92883189101046	0.33516410898329	-4.41095282606674
C	-1.40942341363535	0.32710171151951	-4.21747665403048
N	-1.22538355361127	0.07291549581185	-2.76628817855387
C	-2.52636656361865	-0.21236332104336	-2.11440415389630
C	-0.05857690135497	0.13627950670844	-2.13472412247297
N	1.01962775427496	0.42219469203545	-2.86728442738345
C	2.43531988684526	0.65726877050925	-2.44388076071574
C	2.51889536808021	1.86559698482024	-1.50157208556871
C	3.19470396601994	0.96757389830022	-3.74091221021389
C	3.03137844786732	-0.59782624784585	-1.79628244794461
H	-3.31760584966475	-1.61962473538514	-3.55060316038482
H	-4.49082879402372	-0.39706942871241	-3.04303231386756
H	-3.31301788069594	1.35008836222847	-4.28666348462686
H	-3.21077103920163	-0.01447057826301	-5.40315096599065
H	-0.95176459860608	1.27826858732958	-4.49884987677097
H	-0.93126866053555	-0.47423775387609	-4.78908391178624
H	-2.42048940072747	-1.01584944078084	-1.38885341680564
H	-2.87682584157662	0.68386737885689	-1.59568925029431
H	2.77992140632440	1.84930425862872	-4.23567635675815
H	3.15230753140261	0.12252338789548	-4.43263656789795
H	4.24225388784448	1.16928962841182	-3.51673117171273
H	2.10797394858563	2.75705192758672	-1.97928128560850
H	3.56149634267637	2.06117060361134	-1.24461488883793
H	1.97142445848231	1.69067639494308	-0.57356683394606
H	2.53428590757636	-0.84323500168876	-0.85674045186285
H	4.08808883190436	-0.43055597437182	-1.58079095127954
H	2.94477585741800	-1.45626558851065	-2.46490167229190

H	0.87898173663839	0.56574815083391	-3.85888796465631
Au	-0.00156512327361	-0.14559019705901	-0.08658138259419
Se	-0.12862178237409	-0.17886268966153	2.39195124373484
C	1.53626925415536	-0.95760624411318	2.95593086565663
N	1.95055506451043	-2.13346077316748	2.52742726156607
N	2.23423416246902	-0.29540020140813	3.86316213261437
H	1.95178719731799	0.63035866292914	4.14308291686749
H	3.05711927881389	-0.68968989605037	4.30000897919759
H	1.38469447472952	-2.71189539143127	1.92017035348623
H	2.82261536500862	-2.53425361623522	2.84831962488019
C	1.01435684066798	-7.34859067506951	0.62089305298741
C	0.17113250031785	-7.65654638354948	-0.62376922097039
C	-0.29665324732753	-6.30521674835642	-1.13799341530543
H	-0.70493303610097	-8.27077535182264	-0.41361001152779
H	0.73815660416444	-8.14755786117712	-1.41601589389769
C	1.01074723720104	-5.83606418072060	0.73924738311547
H	2.04638798726795	-7.69134612558126	0.54229638853026
H	0.59552272681924	-7.76662193744518	1.53711010371842
N	0.23785890402840	-5.33188593459128	-0.29606914825824
O	1.56991050115085	-5.15694192174647	1.57755607255513
O	-0.99891391097911	-6.08022342732125	-2.09691544770243
I	-0.06705248549436	-3.25438333662463	-0.50267850455842

50

1A3TS

C	-0.45221604942503	-0.29733730429972	1.99946470183033
N	-1.63333360990493	-0.86594384129173	2.55140786133811
C	-2.85369625690620	-0.04347394890879	2.37054594758957

C	-3.98401397351205	-1.00340835334491	2.77566665478197
C	-3.40369180862043	-2.42303650958428	2.54354145548659
C	-1.99874630755576	-2.18399054089758	1.97332991903032
N	0.45515282906377	-0.09955269550783	2.90460250623382
C	1.86682147280208	0.41124936623210	2.80904709277759
C	2.70523978590603	-0.57727869538582	1.98945337148936
C	2.37367343010059	0.46449052092256	4.25510460186009
C	1.88503227343150	1.81421891398308	2.19464956453502
H	-4.24936726232443	-0.86267515832657	3.82316115480741
H	-4.87609290316759	-0.81505491875582	2.17904773951827
H	-4.00531341274043	-3.01710873744518	1.85521226564725
H	-3.34003844334527	-2.96846690254439	3.48524876291548
H	-2.02821205443373	-2.12919836162424	0.87540405634564
H	-1.27203988879495	-2.94276434259771	2.26338816788115
H	-2.80041572073592	0.85790440919451	2.97958004531520
H	-2.96497220260324	0.25129679008683	1.31704685646433
H	2.34442437671500	-0.52409115743254	4.71946123242523
H	1.77552723126465	1.15351243506157	4.85485232507784
H	3.40636223556791	0.81228020068814	4.26535278403152
H	2.67607786865832	-1.57408100498852	2.43320243159085
H	3.74208067583452	-0.23837393043483	1.97078478517675
H	2.34859059662165	-0.64445648482517	0.96057864860677
H	1.53741623881638	1.80452849910663	1.16172524704396
H	2.90821587429118	2.19291132088901	2.20496202086266
H	1.25648039308391	2.49846831819461	2.76653358288608
H	0.16488715234195	-0.37853230296720	3.84184071301560
Au	-0.23614088506589	0.02887214926128	-0.01419323960446
Se	0.05358788852072	0.07010882329084	-2.48463766980891
C	1.56234452344119	1.24616858649701	-2.71551978086718

N	1.50146795431813	2.52972703395197	-2.42272774362967
N	2.65665871421839	0.73442475702091	-3.25180949916127
H	2.71171085736035	-0.25369709072005	-3.44149796659273
H	3.45313007163026	1.30667221045269	-3.50087638263164
H	0.64589214445219	2.97489067321606	-2.11198818420379
H	2.28711040843817	3.14554176852171	-2.59170822378137
C	-1.38857510644283	7.11116444368789	-1.57397770215864
C	-2.49139368287634	7.29882301960805	-0.52373178593880
C	-2.71772519273336	5.92150116187950	0.07506962099559
H	-3.43183355580124	7.66296124699107	-0.93715014081115
H	-2.20035772816705	7.97398091778941	0.28243485725307
C	-0.97229294346538	5.65840465975655	-1.45790682227407
H	-0.51618190651818	7.74499135018399	-1.41309927798640
H	-1.73868850298302	7.28282505131985	-2.59319165922229
N	-1.79099775102068	5.05815842042108	-0.51377293464282
O	-0.09063389184841	5.08661449183769	-2.06902868146963
O	-3.52379799619172	5.59872448232450	0.91519174924272
I	-1.57611595969476	3.02710625951184	-0.04707502927130

5

A1

C	-1.17999963809415	-3.13264705701285	1.34122210040500
F	-0.35509176300000	-4.18370212052023	1.36935783914215
F	-1.52209115059930	-2.83433355861292	2.59821333346661
F	-2.28581333752348	-3.48562798371543	0.67845788966677
I	-0.22172411078307	-1.42735928013857	0.37943883731948

8

A2

C	5.58286908707159	0.05969435877283	2.74475293343128
C	6.37854300613514	0.82557557220609	1.64507810027923
I	3.43098231409612	0.05118147028205	2.37589055811576
F	5.84074418104458	0.64453664734399	3.92912299509035
F	6.04442839677838	-1.20318665905530	2.79048956389622
F	5.99599546584372	2.10435930516140	1.59033695423526
F	6.19184429249963	0.26132621808391	0.44826944018823
F	7.68692325653084	0.78524308720504	1.93396945476366

12

A3

C	0.98748915048958	-7.03894255805765	0.29963094248694
C	-0.04719747210382	-7.28738545640659	-0.80452763012722
C	-0.53901538595405	-5.91291129146767	-1.21778292779878
H	-0.90491620648442	-7.87093999390260	-0.46777504365204
H	0.36719207595456	-7.78358570289632	-1.68276943648768
C	1.03365009536270	-5.53387197263789	0.48312937991180
H	1.98854220305044	-7.38275837908400	0.03695142213751
H	0.72032751648439	-7.49498950316449	1.25338960432427
N	0.13098758820774	-4.97702974947257	-0.42611731783281
O	1.71186008295678	-4.90380418590811	1.25965577039869
O	-1.35652327530184	-5.64375003581310	-2.06585778251815

I -0.18270637266205 -2.94163117118901 -0.58896698084253

8

SeU

Se	0.29132366926730	0.24128276302062	2.02237246455948
C	0.10331258911759	2.05846318964385	2.42256853270624
N	1.13994145728390	2.78235231423585	2.85542483794854
N	-1.07156217983621	2.67989837612849	2.28281653597660
H	-1.86824092848761	2.15917978499174	1.95749683956973
H	-1.19844383229798	3.65738044686920	2.50302571769675
H	2.03146364367554	2.33557766144497	2.98752706568377
H	1.05708558127747	3.76031546366527	3.09322800585888

74

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Au	0.66684892497884	7.83724788237557	5.50105034364353
Se	2.09800632256441	6.29862480698398	4.21088027991519
N	2.35809676933045	6.13980189154544	1.45106445561944
H	3.00483944599426	5.39969933343794	1.67369967137886
H	2.21112735977596	6.35146605694226	0.47377785154583
N	0.88135053497886	7.76683825177220	2.09837270933497
H	0.69483420735086	8.02165254484104	1.13789070942683
H	0.40380864920539	8.27363340786428	2.82708511317839

N	-0.63450713675679	9.19140303543642	7.92555206993544
N	-1.34145455632551	10.04677903432292	6.07942435683779
C	1.72971184732063	6.79917994775725	2.41349224996265
C	-0.50708869302715	9.10207992926193	6.57954045313168
C	-1.98674093895617	10.72175503969393	7.10578379545115
H	-2.69141672029297	11.51155799459404	6.91503631233742
C	-1.54299309396198	10.18446347790693	8.26432184819717
H	-1.78454717806348	10.41198632566462	9.28732128360974
C	-1.52424685090973	10.32269025231949	4.67087881980118
C	-0.68611901229344	11.27091914042381	4.05842406729032
C	-0.88102015057305	11.51288743750980	2.69682451672635
H	-0.25522854299115	12.23684515720516	2.18985031475659
C	-1.87001634562550	10.84848449807808	1.98386294632332
H	-2.00680111119173	11.05624228240119	0.92918776755294
C	-2.69163337497941	9.92750181730708	2.61969468901316
H	-3.46689646808080	9.42662042183358	2.05340712373722
C	-2.54268824680353	9.64446919287508	3.97930779030059
C	0.38982715731707	12.03903852024549	4.81466988041803
H	0.40398546311217	11.68160071526902	5.84404343496734
C	1.78978730671082	11.79056777017282	4.23006365479071
H	1.86509279003855	12.15261197082716	3.20220694497360
H	2.03932912298501	10.72739375786917	4.23413342298160
H	2.54122631536763	12.31648393149034	4.82299575720090
C	0.07008666188247	13.54328306004975	4.85951065267818
H	-0.91446561832926	13.72946729624214	5.29431786272492
H	0.08398432647521	13.98319105622022	3.85943760772969
H	0.81297867746210	14.06656270007148	5.46568429529586
C	-3.47534767744277	8.64311106892996	4.64759888169614
H	-3.18147451108203	8.54721732408229	5.69289453583037

C	-4.93160630668115	9.13980982798008	4.62941279404482
H	-5.31029913885667	9.22522591191813	3.60817198051362
H	-5.02285716592120	10.11835261355797	5.10565827000434
H	-5.57357993855589	8.43901994167212	5.16769920189583
C	-3.36027665560213	7.24597702614287	4.01485533450027
H	-3.99620672984568	6.53858776173285	4.55163700443133
H	-2.33341116628821	6.87528522913325	4.05467329394104
H	-3.67799887358954	7.25368762184093	2.96995842669844
C	0.07543857491972	8.37365842354452	8.88685136676271
C	1.30750497571081	8.83585278002316	9.37886648558475
C	1.96589874979842	8.03299628185035	10.31232063385872
H	2.91891687524403	8.35437260210500	10.71244255545971
C	1.41796750905011	6.83089463047408	10.73760782971576
H	1.94621616118625	6.22349929532771	11.46298816222343
C	0.19394912609261	6.40562111544460	10.24050529260231
H	-0.22243535194528	5.46760720104104	10.58496116382729
C	-0.51017519971003	7.16751244525383	9.30578824893188
C	1.93583587011209	10.15254592496651	8.94137717065028
H	1.27088668158316	10.62330044188311	8.21647773883899
C	3.28543137286622	9.92967244518993	8.23786156583261
H	3.17818158286839	9.26174959250384	7.38044308069761
H	4.02229188386456	9.49355776750586	8.91606909557214
H	3.68379712723782	10.88190024590286	7.87993326458204
C	2.07952843255647	11.12830777885230	10.12182572192024
H	2.76838183494973	10.74263497502207	10.87692980332577
H	1.11735753129059	11.31151426113978	10.60539813114708
H	2.46997158793267	12.08624816440986	9.77122975133712
C	-1.85525220433800	6.67286423377256	8.79066198451437
H	-2.24487171887229	7.41162940371091	8.08950202803989

C	-1.71218496739661	5.34906380092963	8.02095165566868
H	-1.35137362683815	4.54795986005126	8.66999032005901
H	-1.01310785948497	5.45032636326320	7.18803735386108
H	-2.68006983405155	5.04200898894621	7.61775870854327
C	-2.88232491071664	6.54498819498847	9.92850950039517
H	-3.85431220262695	6.25260521250551	9.52472134760601
H	-3.00694567714783	7.49112985235896	10.46021704911825
H	-2.58043500395917	5.78695945123088	10.65450521299890

86

2A3

Au	-0.64192632476325	2.15258755385499	-0.69733641224844
Se	-0.07469114950588	-0.25421789137920	-0.67746065004260
N	-1.81428732857565	-2.41597797502323	-0.41686162615483
H	-0.96024876776195	-2.94811308534189	-0.50389669163323
H	-2.67445025175139	-2.93524213759988	-0.28123347910105
N	-2.91305045322323	-0.40141122417743	-0.31047277481473
H	-3.80941045732410	-0.85411341365335	-0.16777864218651
H	-2.89029407873369	0.60977261145280	-0.32317061639547
N	-0.33694315150878	5.26670967442735	-0.56230914414635
N	-2.39464659322206	4.64073194337763	-0.58733247738143
C	-1.79522292001212	-1.09425813915746	-0.43939028424699
C	-1.12424489338307	4.16064307379229	-0.58257144348585
C	-2.40180021441697	6.02670121913206	-0.59101719480905
H	-3.31516115228232	6.59307067966313	-0.59455524124269
C	-1.10908905810459	6.41992247995074	-0.57724927761847
H	-0.66703955865176	7.40063554084907	-0.57178132626847

C	-3.58466650963141	3.82997008731354	-0.48162966203331
C	-4.15904119361369	3.32512089357184	-1.65071083783642
C	-5.29073728874613	2.51399042554595	-1.50553380220820
H	-5.76719411878429	2.10806576789830	-2.38279958707860
C	-5.81831205841711	2.23688014760493	-0.25106902453903
H	-6.69406613712008	1.60765003287491	-0.15887789895436
C	-5.23985874262459	2.77749533375599	0.88600009199096
H	-5.67438765250274	2.56588173885793	1.85515308090057
C	-4.11528000379126	3.59892301967409	0.80030836404708
C	-3.61905606407844	3.68036890467634	-3.02649295443213
H	-2.69461933249408	4.24076953195300	-2.88917463398653
C	-3.27704039185663	2.44668405051967	-3.86929124944132
H	-4.16792306575084	1.86095343694137	-4.10958069200846
H	-2.57283289429145	1.79651633931982	-3.35270390563226
H	-2.81798206799288	2.75928832210778	-4.80760841782788
C	-4.59518326340326	4.60790334340739	-3.75960080078942
H	-4.85218913983291	5.47689603582545	-3.15243171264163
H	-5.52094560470648	4.08517232360845	-4.00781470817832
H	-4.14615539034568	4.96665350599010	-4.68765443327844
C	-3.52115722711847	4.21678314855666	2.05932472544562
H	-2.68492238658320	4.84826438718797	1.76404571685722
C	-4.53314501979036	5.13196388240231	2.77226214440748
H	-5.37214408846285	4.56236674439520	3.17402984127468
H	-4.93414896565182	5.89592390505328	2.10120025627812
H	-4.04319653638844	5.63768238271778	3.60614418291124
C	-2.96723825306921	3.15357498610839	3.01696559535684
H	-2.49815552272189	3.63643449005078	3.87576988590827
H	-2.21635381547448	2.53060687257587	2.52474229702460
H	-3.75652274991977	2.50178582914992	3.39379898299379

C	1.10366991987691	5.30048770117904	-0.44099941363351
C	1.87922791792176	5.23707033431628	-1.60630068843562
C	3.25995731553024	5.32342999567759	-1.45857596981912
H	3.89135171872929	5.27159402288805	-2.33468604832125
C	3.83444155356377	5.48480513334307	-0.20946944173345
H	4.90734260406090	5.55729295012072	-0.11805212550242
C	3.03927107306533	5.56818410574504	0.92319828804309
H	3.50370837800345	5.71652294909369	1.88706389629538
C	1.65327118904296	5.48844754585762	0.83833873631572
C	1.27709073908842	5.10431871126638	-2.99403775790973
H	0.19977730354078	5.01105692470048	-2.88957627650709
C	1.76936393339884	3.84067011159796	-3.71128448843604
H	1.55813768272991	2.95022499687074	-3.12181497563316
H	2.84223918614777	3.87932409819910	-3.89401722287679
H	1.26845985106986	3.73617721318790	-4.67309945794239
C	1.54231529108529	6.36366866332798	-3.82909869680728
H	2.60713010572025	6.50546783401136	-4.01083429983878
H	1.16716710811200	7.25592492039009	-3.32581365732682
H	1.04221069258525	6.28385830971529	-4.79487277389527
C	0.80888472236232	5.66921467994612	2.09278725205276
H	-0.23286735989122	5.49824883022766	1.82686814198355
C	1.15832866077595	4.66230809170723	3.20142525276648
H	2.19319850336407	4.77115597595814	3.52934539602047
H	1.00874071888125	3.63234419541039	2.86540055055255
H	0.52036149163659	4.82968907361306	4.06987903540020
C	0.91380174011455	7.11522541058858	2.61869682111987
H	0.24218425433497	7.25474350845534	3.46561098207347
H	0.64705484209813	7.84583490747617	1.84909801212908
H	1.92605747753804	7.34025102994006	2.95823883843622

C	-0.42947426693720	0.59982641811889	5.41959020657981
H	-0.46670722211136	1.89568535693980	7.11440603838337
H	-0.09895874191279	0.22139289709927	7.48615486043664
C	1.82279456986637	1.08022433567606	5.07989692250965
H	2.23149103397061	0.63749834971263	7.10814516032275
H	1.87969655180420	2.32386719727526	6.81986426981963
N	0.62095368574403	0.66909961322291	4.51349322092626
O	2.87648100886197	1.20119081925069	4.48189448592972
O	-1.57000406827341	0.27575663642754	5.14599473744004
C	1.58565873074570	1.30771660223156	6.56116925025149
C	0.09502054905403	1.02288345116324	6.77801407845306
I	0.38637139308558	0.22816531825817	2.44551529762340

31

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C	-4.12172910511943	-0.05171938409614	-3.14548687619003
C	-5.01804780676703	-0.66450654692927	-4.22794830193169
C	-4.02360178472966	-1.30921496888582	-5.19902180982581
N	-2.78397388952965	-0.51448325394771	-5.03699273760560
C	-2.92607453432094	0.46978432772756	-3.94044501133822
C	-1.68392724840325	-0.66224881845347	-5.77531271539118
N	-1.72612244229185	-1.60684316024242	-6.72177007449732
C	-0.67639994828104	-2.02661681941840	-7.69907875094737
C	-0.32201806983044	-0.87062848718780	-8.64415284753082
C	-1.31299946166774	-3.16784007310817	-8.50429633323179
C	0.56866068633274	-2.54911334560250	-6.96979875598533

H	-3.79661483639864	-0.82084463409115	-2.44046042302866
H	-4.61371543080742	0.74134629231614	-2.58306803809841
H	-5.58108730240302	0.11982631694457	-4.73853376616826
H	-5.72995105887246	-1.39152075295981	-3.83743173514280
H	-4.37390312442875	-1.27158140703139	-6.23368912788494
H	-3.82486441866177	-2.35414340087561	-4.93862951240487
H	-2.00687271270952	0.52155562652171	-3.36140639220981
H	-3.13073724818468	1.45913450595286	-4.35945218165766
H	-2.20964246993171	-2.82575883418952	-9.02744436048748
H	-1.58277334922912	-4.00340231236567	-7.85370059410483
H	-0.60726588882494	-3.53486084022027	-9.25001382533252
H	-1.21229969204600	-0.51557680228438	-9.16748000449629
H	0.40440820215849	-1.21021323380336	-9.38530125380936
H	0.11510475955855	-0.03273236244871	-8.09972736216614
H	1.04312500123447	-1.76268116866075	-6.38123760679054
H	1.29502945635771	-2.91168065905913	-7.69966325198824
H	0.30639386181809	-3.37128720904050	-6.30068296536779
H	-2.58135465448645	-2.13818806263663	-6.81245466691092
Au	-0.07076487856877	0.52224773672593	-5.43121404630814
Cl	1.78501938903424	1.89479173134981	-5.00910467116720

31

3TS

Au	-0.19047824466350	0.30464009989539	-0.01272106434452
C	-0.02775604402708	0.15881683102168	1.97357718173697
N	0.19018504672474	-1.08486331064713	2.65330388605579
C	-0.85464062769373	-2.10090849661841	2.38811735301324

C	-0.24068501053451	-3.37600402227634	2.97732455247871
C	1.28938039507643	-3.18366486526380	2.81490549130158
C	1.45471262609600	-1.75616488708460	2.26372788906717
N	-0.08574436852255	1.13482044958182	2.84181009710249
C	-0.29682152998085	2.60545887644552	2.64714204913906
C	0.83805456421697	3.18961728948949	1.79678267570959
C	-0.26544909982816	3.21078265713178	4.05639421348522
C	-1.66467269889113	2.85486081135625	1.99834887804643
H	-0.50321094597033	-3.46887597363044	4.03163870391458
H	-0.61110893019053	-4.26392570937368	2.46483238546219
H	1.72660445608290	-3.90971296524248	2.12922659127155
H	1.79687905170519	-3.29144642949116	3.77348388211961
H	1.56427534712948	-1.76739881526050	1.17102278989176
H	2.30844878865342	-1.22538988868193	2.68624219972758
H	-1.79370035366265	-1.81236080833964	2.86086738329060
H	-1.03021632914764	-2.20789827650742	1.30886656290220
H	0.69839780202047	3.03850263031584	4.54344248558945
H	-1.05625380883393	2.79318161516069	4.68506741125264
H	-0.42022513397082	4.28823910522357	3.99800833238585
H	1.81043435163126	2.98478859829895	2.25006527303258
H	0.71529019278410	4.27174035388480	1.72153677646841
H	0.83045341464224	2.77305203689480	0.79004585645073
H	-1.71308685571869	2.42098240655570	1.00016196305013
H	-1.83537006536381	3.92966550908122	1.91437441813727
H	-2.46678498291337	2.42598082864659	2.60268563216642
H	0.02784565955215	0.82718823058406	3.80625107115912
Cl	-0.34414444368600	0.44532039660897	-2.31168066523662

43

3A3

C	-2.82814833864466	-0.63582328030008	-3.14796692121810
C	-2.37381275938125	-0.26831405282663	-4.56575362165608
C	-0.84640725304980	-0.35387901749581	-4.48778827003378
N	-0.53604844680812	-0.06323940595354	-3.06850005539873
C	-1.77682699637105	0.03143827189049	-2.26344305881123
C	0.69217613650305	0.08722565917301	-2.57641720675717
N	1.70587633937261	-0.05308226084558	-3.43633894733988
C	3.17845385250286	0.05013075216181	-3.20288783667744
C	3.55465428395868	1.46268009555124	-2.73601401365410
C	3.82144549895590	-0.22440236005843	-4.56953410361511
C	3.64680197483915	-1.01091327037092	-2.19826871139777
H	-2.80191180941495	-1.71926971233066	-3.00831213079284
H	-3.83398097285880	-0.28608008427578	-2.91771350590067
H	-2.67679686547848	0.75338234005256	-4.80434043966407
H	-2.77714968003666	-0.92850403933310	-5.33284215252299
H	-0.35786145452843	0.37051664150887	-5.14398865094119
H	-0.48450814205250	-1.35463210624828	-4.74386963707195
H	-1.63934428255702	-0.46290034436948	-1.30441332190392
H	-2.01800079730855	1.08224627667435	-2.08407844673462
H	3.49562501062497	0.50862261349864	-5.31216117081467
H	3.56614335065171	-1.22499347542534	-4.92783475290333
H	4.90680042753563	-0.16246104597081	-4.48630593108194
H	3.21883875667379	2.20982894714469	-3.45828362204454

H	4.63911599420067	1.53982303725929	-2.63552280617570
H	3.10801636316181	1.69385267993148	-1.76804528035641
H	3.19936331008142	-0.85704218989945	-1.21560717121090
H	4.73193111262544	-0.95790138972472	-2.08770096203808
H	3.38276057881770	-2.01227678992290	-2.54535045840737
H	1.47410587712713	-0.27167889426791	-4.39587225715369
Au	0.93204026290326	0.51024665589899	-0.60646292571905
Cl	1.17570077262450	0.99119028258910	1.69345034566050
I	-0.33874952495197	-1.24280161360729	3.07097787591847
N	-1.38964660413318	-2.78557052707052	4.06039761343237
C	-0.81444258257014	-3.59254047679646	5.03609797501970
C	-1.86850243183360	-4.57838586070612	5.51144994178330
C	-3.12579349235290	-4.24006145352481	4.70546829100428
C	-2.72018541378773	-3.08975827623561	3.79850170671067
H	-1.50004854934746	-5.58974299182142	5.33335460713193
H	-1.99675665835745	-4.45795047538537	6.58796714194580
H	-3.96100233463950	-3.91186664986609	5.32580918749332
H	-3.47900662355130	-5.06447021802652	4.08512445314995
O	0.33057294428586	-3.50839356819635	5.42422659277506
O	-3.41949083343062	-2.52324842247853	2.98579263797198

43

3A3TS

C	-0.120430	0.056897	2.107794
N	0.189408	-1.184210	2.735481
C	-0.728915	-2.291554	2.372709
C	-0.001445	-3.535812	2.905137
C	1.498436	-3.140626	2.932675

C	1.538356	-1.703662	2.394462
N	-0.260858	1.009296	2.980369
C	-0.555636	2.473361	2.814591
C	0.595720	3.144580	2.056264
C	-0.643436	3.029229	4.241211
C	-1.895761	2.666061	2.094569
H	-0.350916	-3.782888	3.907404
H	-0.194409	-4.396290	2.264494
H	2.116485	-3.798708	2.321779
H	1.884363	-3.174529	3.951770
H	1.690862	-1.697167	1.306094
H	2.309602	-1.086224	2.854870
H	-1.708277	-2.131608	2.823064
H	-0.853848	-2.348854	1.282489
H	0.293920	2.875611	4.781673
H	-1.453841	2.553471	4.797785
H	-0.839834	4.100646	4.202713
H	1.541757	3.002380	2.582483
H	0.399274	4.214875	1.977278
H	0.693115	2.742121	1.048065
H	-1.854872	2.309543	1.065403
H	-2.138296	3.729761	2.077435
H	-2.694955	2.137015	2.616657
H	-0.133673	0.703958	3.944446
Au	-0.283109	0.235597	0.111069
Cl	-0.486035	0.355494	-2.241706
I	1.103624	2.830630	-3.079335
N	2.175997	4.538775	-3.697526
C	3.365089	4.471758	-4.416251

C	3.813612	5.893020	-4.712977
C	2.751289	6.791239	-4.071582
C	1.747703	5.837254	-3.446270
H	4.811327	6.035202	-4.296904
H	3.885404	6.014095	-5.794730
H	2.226857	7.420874	-4.792151
H	3.145796	7.440376	-3.289421
O	3.921083	3.448007	-4.749632
O	0.742318	6.134855	-2.837749