Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

The Structures and Properties of Proton- and Alkali-bound Cysteine Dimers

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Thermochemistry

As determined with harmonic frequency calculations at the B3LYP/6-311++G(d,p) level of theory.

$Cys_2 \bullet H^+$

Isomer	H kJ•mol^{-1}	S kJ•mol^{-1}•K^{-1}	G° kJ•mol^{-1}
Global Minimum	0.0	0.62	0.0
Isomer 5	12.0	0.60	17.5
Isomer 10	18.0	0.62	17.2

$Cys_2 \bullet Li^+$

Isomer	H kJ•mol^{-1}	S kJ•mol^{-1}•K^{-1}	G° kJ•mol^{-1}
Global Minimum	0.0	0.63	1.1
Isomer 3	2.7	0.64	0.0
Isomer 4	4.1	0.62	8.4
Isomer 8	9.7	0.62	11.9

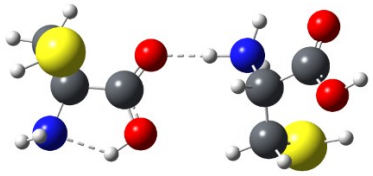
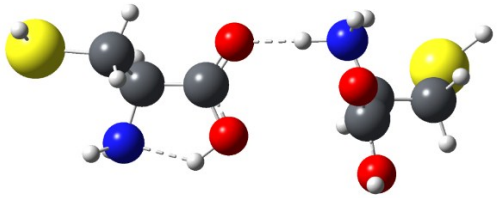
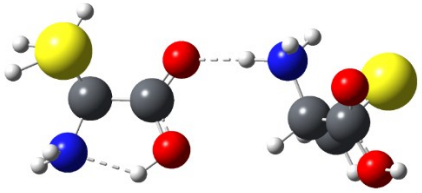
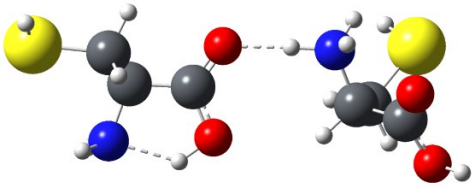
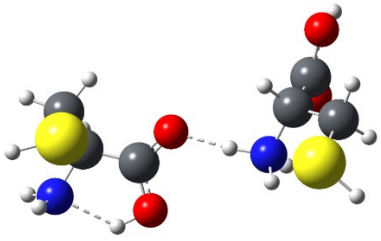
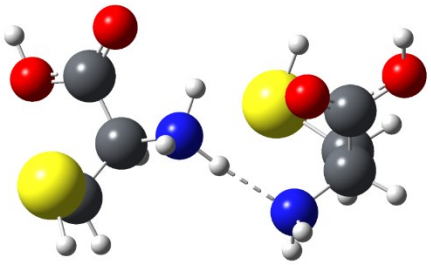
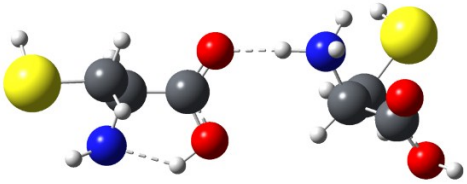
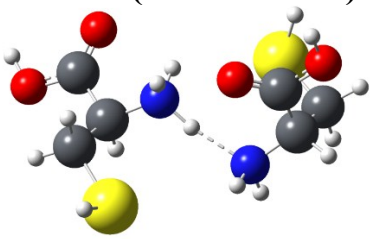
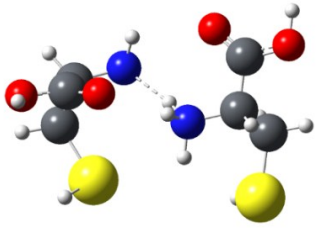
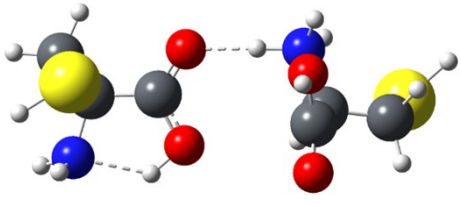
$Cys_2 \bullet Na^+$

Isomer	H kJ•mol^{-1}	S kJ•mol^{-1}•K^{-1}	G° kJ•mol^{-1}
Global Minimum	0.0	0.64	3.9
Isomer 4	4.1	0.65	6.2
Isomer 5	4.8	0.67	0.0
Isomer 9	11.0	0.68	3.3

Conformations and Spectra of $[(Cys)_2M]^+$

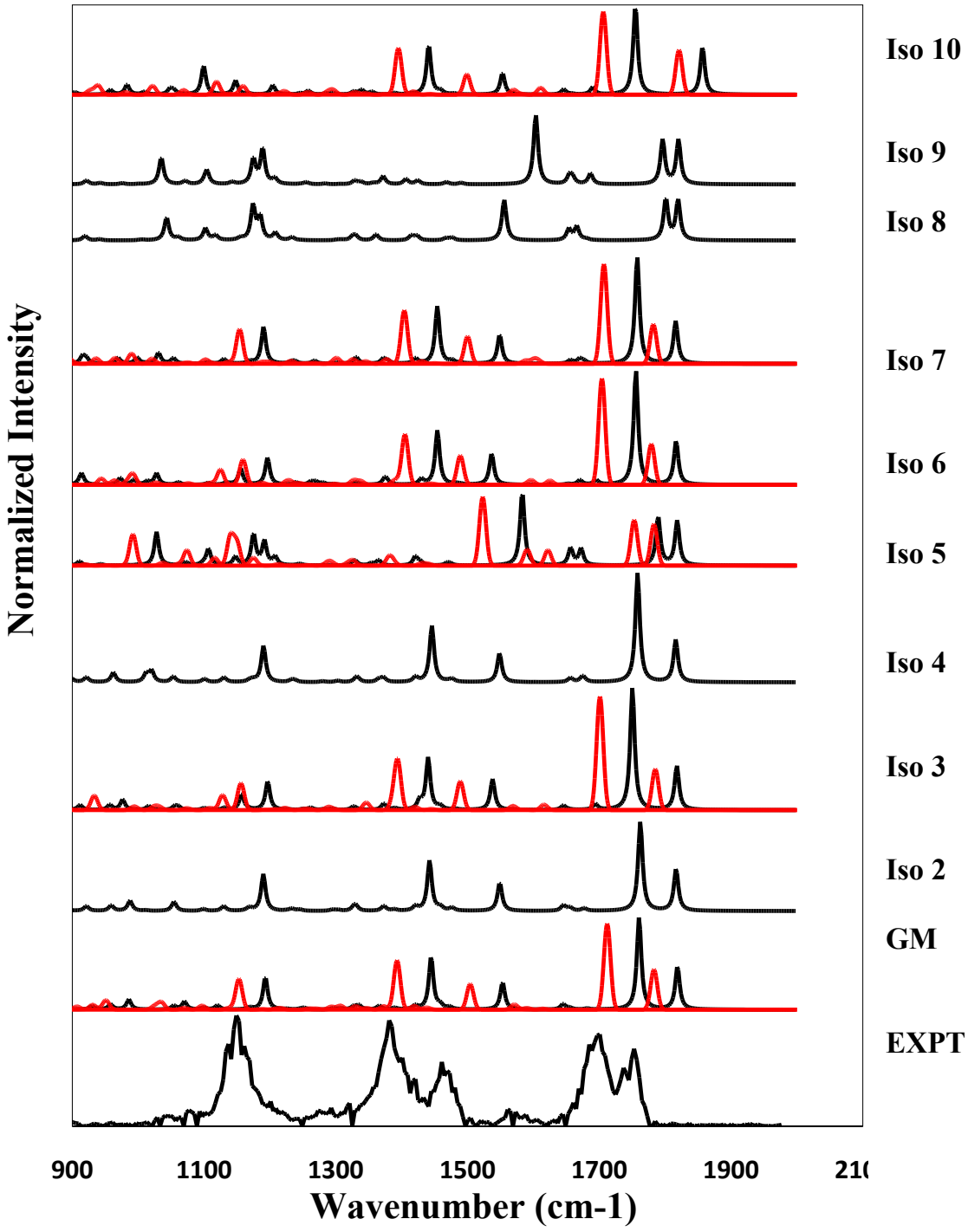
Conformations of Isomers 1-10 of $[(Cys)_2H]^+$

Note: Energies include thermal correction at 298 K

GM	**Iso 6 (13.33 kJ/mol)**
	
Iso 2 (6.40 kJ/mol)	**Iso 7 (13.54 kJ/mol)**
	
Iso 3 (7.43 kJ/mol)	**Iso 8 (16.92 kJ/mol)**
	
Iso 4 (9.69 kJ/mol)	**Iso 9 (17.08 kJ/mol)**
	
Iso 5 (12.01 kJ/mol)	**Iso 10 (17.98 kJ/mol)**
	

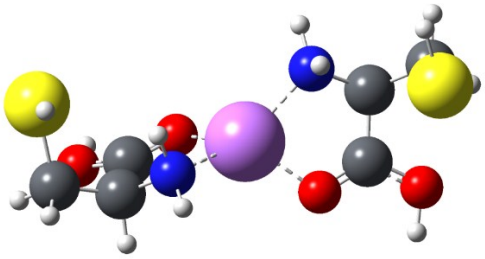
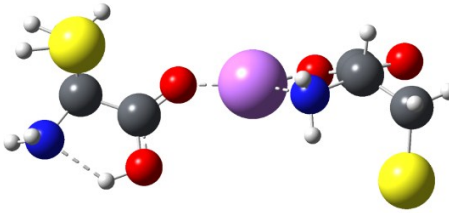
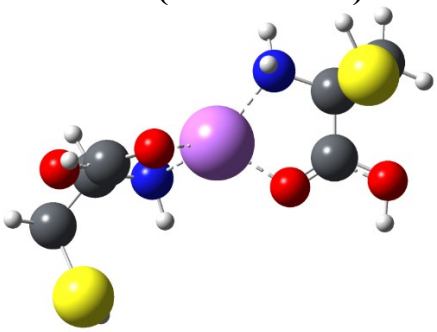
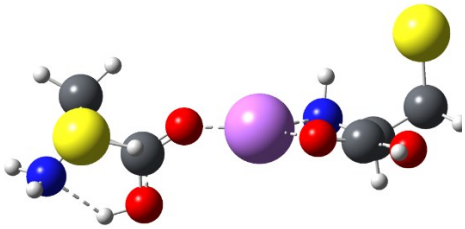
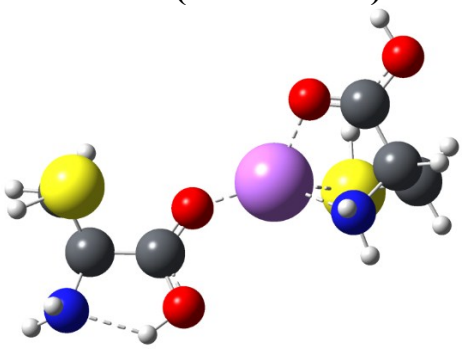
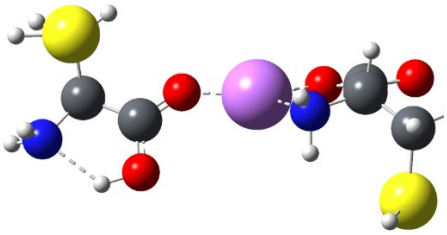
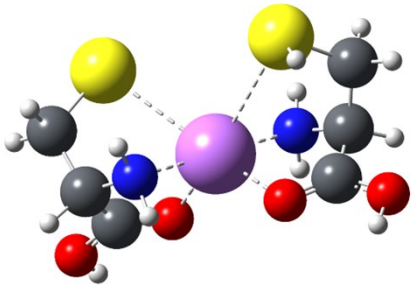
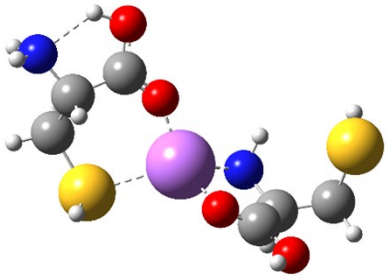
Predicted IR Spectra of Isomers 1-10 of $[(Cys)_2H]^+$

For all following figures, **anharmonic corrections** are shown in **red**.



Conformations of Isomers 1-8 of $[(Cys)_2Li]^+$

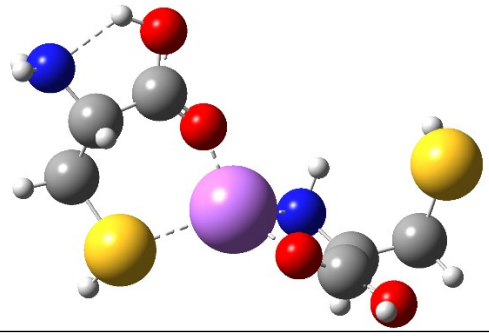
Note: Energies include thermal correction at 298 K

GM	**Iso 5 (5.54 kJ/mol)**
	
Iso 2 (1.27 kJ/mol)	**Iso 6 (8.22 kJ/mol)**
	
Iso 3 (2.74 kJ/mol)	**Iso 7 (9.57 kJ/mol)**
	
Iso 4 (4.12 kJ/mol)	**Iso 8 (9.73 kJ/mol)**
	

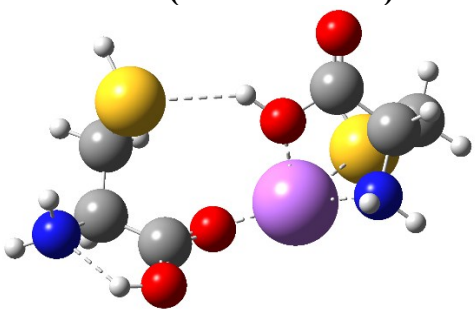
Conformations of Isomers 9-16 of $[(Cys)_2Li]^+$

Note: Energies include thermal correction at 298 K

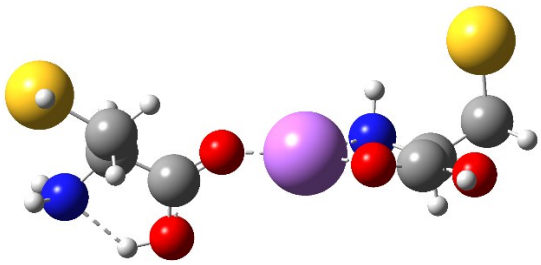
Iso 9 (13.92 kJ/mol)



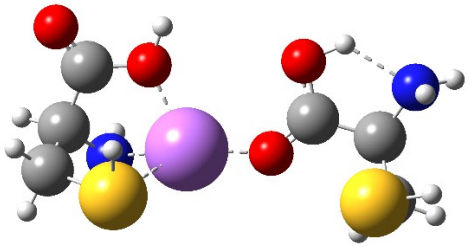
Iso 13 (22.92 kJ/mol)



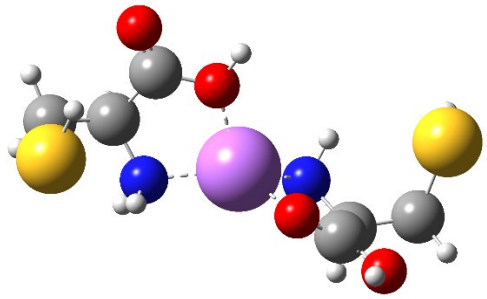
Iso 10 (15.98 kJ/mol)



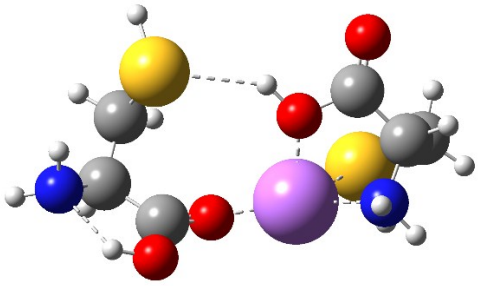
Iso 14 (23.59 kJ/mol)



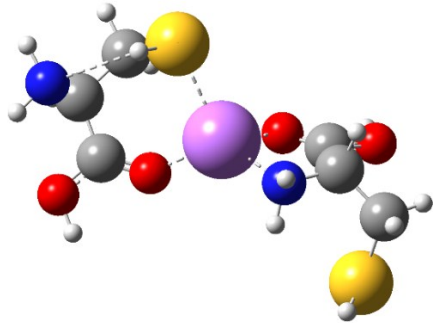
Iso 11 (20.75 kJ/mol)



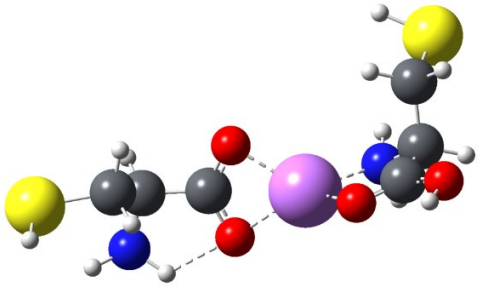
Iso 15 (25.52 kJ/mol)



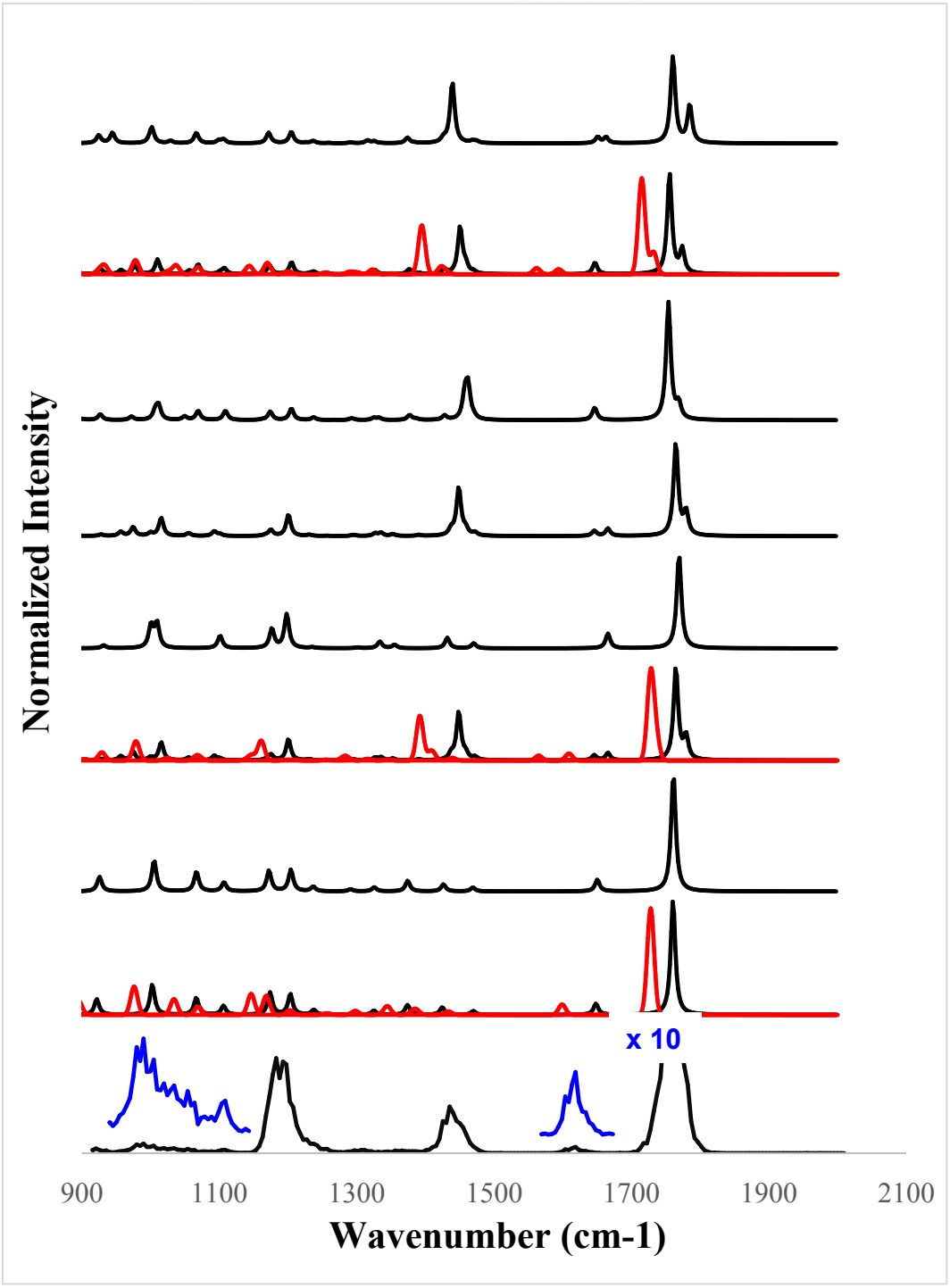
Iso 12 (22.26 kJ/mol)



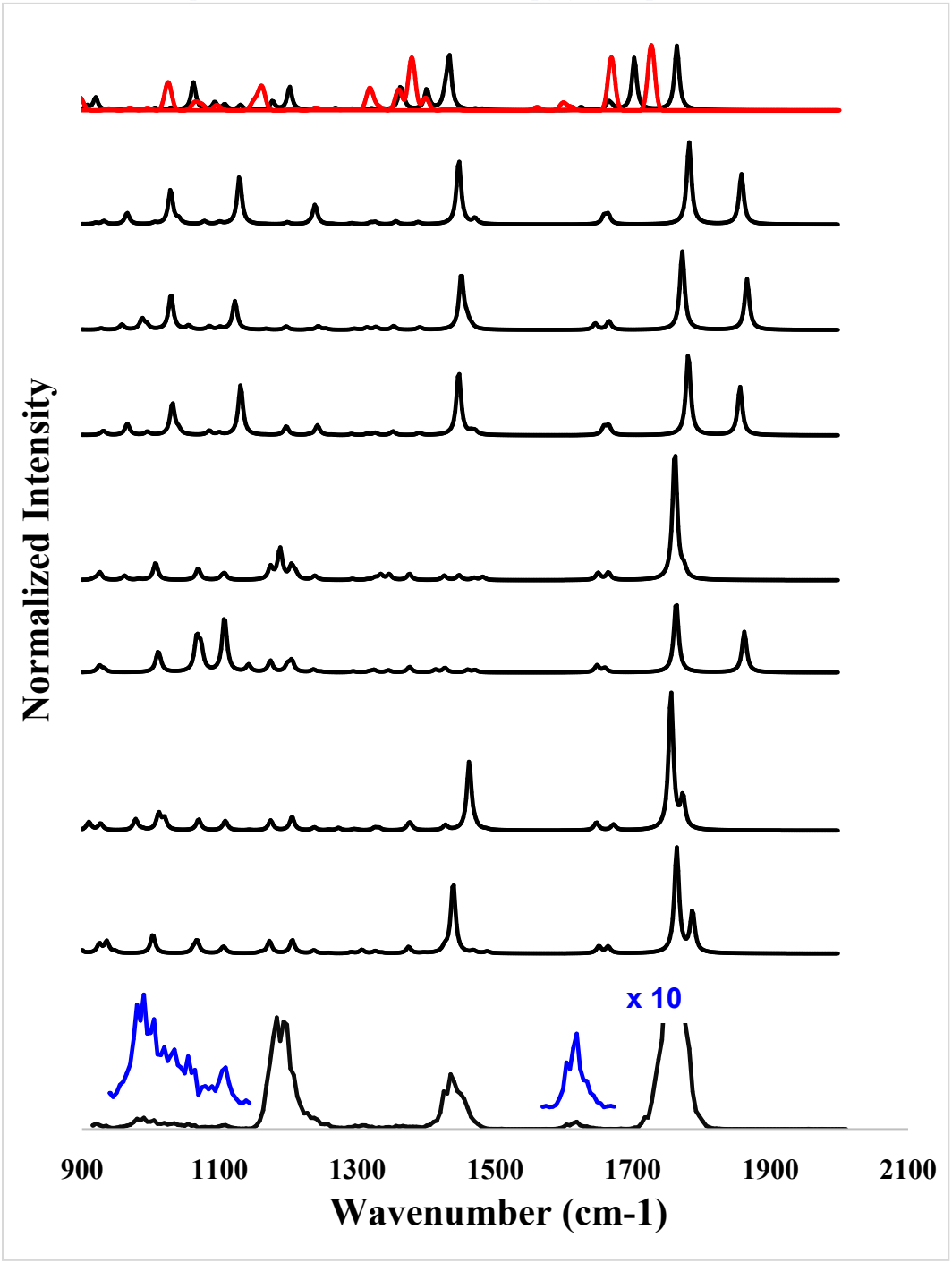
Iso 16 (ZW GM) (25.54 kJ/mol)



Predicted IR Spectra of Isomers 1-8 of $[(Cys)_2Li]^+$

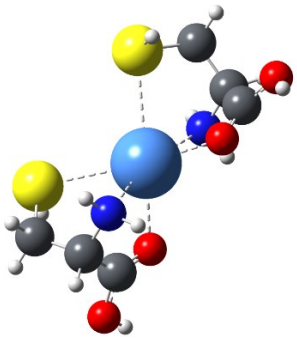
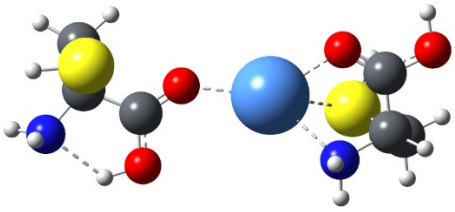
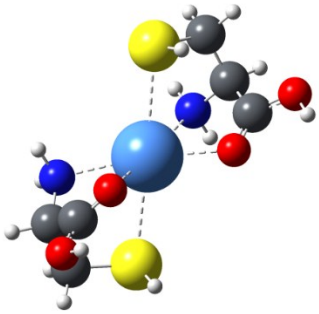
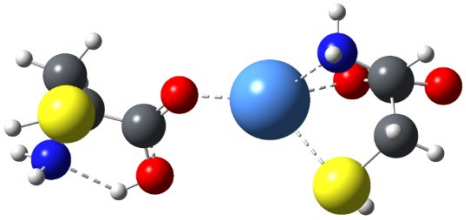
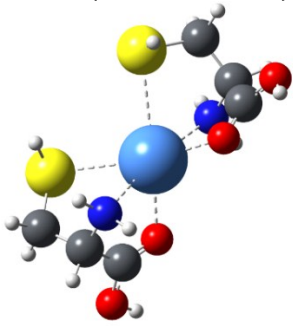
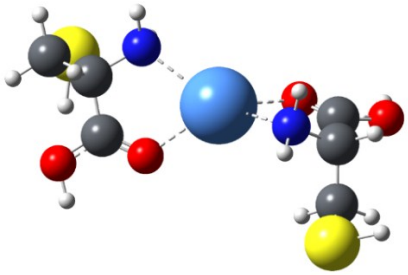
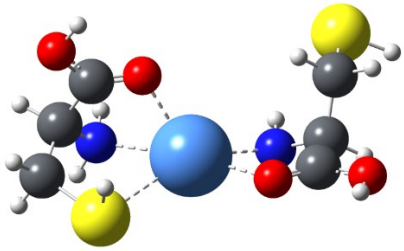
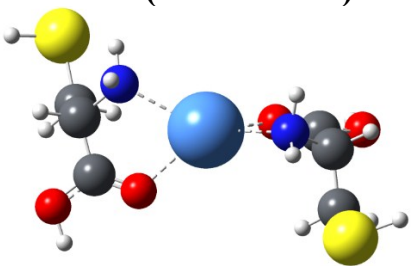


Predicted IR Spectra of Isomers 9-16 of $[(Cys)_2Li]^+$



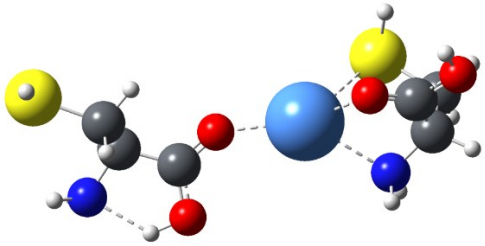
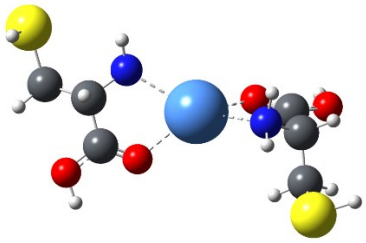
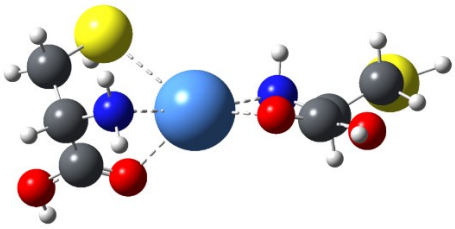
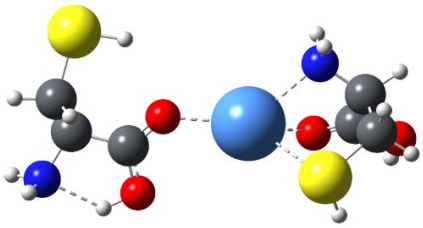
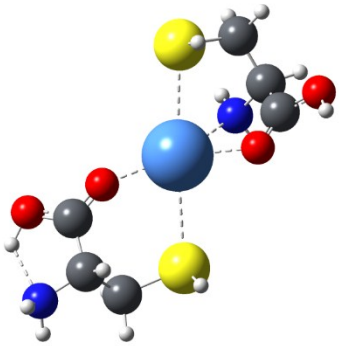
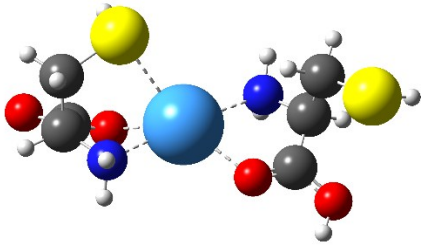
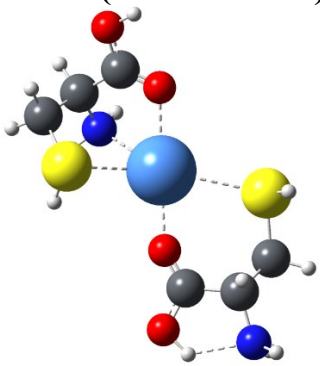
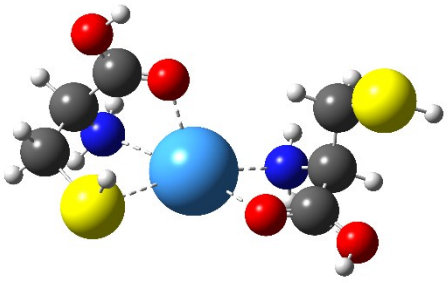
Conformations of Isomers 1-8 of $[(Cys)^2Na]^+$

Note: Energies include thermal correction at 298 K

GM	**Iso 5 (4.82 kJ/mol)**
	
Iso 2 (0.13 kJ/mol)	**Iso 6 (4.88 kJ/mol)**
	
Iso 3 (2.62 kJ/mol)	**Iso 7 (7.62 kJ/mol)**
	
Iso 4 (4.15 kJ/mol)	**Iso 8 (8.77 kJ/mol)**
	

Conformations of Isomers 9-16 of $[(Cys)_2Na]^+$

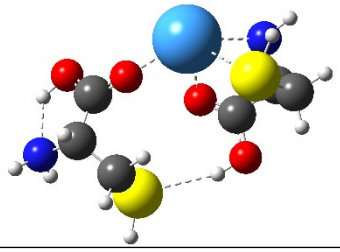
Note: Energies include thermal correction at 298 K

Iso 9 (10.95 kJ/mol)	**Iso 13 (13.32 kJ/mol)**
	
Iso 10 (12.79 kJ/mol)	**Iso 14 (16.43 kJ/mol)**
	
Iso 11 (12.99 kJ/mol)	**Iso 15 (17.35 kJ/mol)**
	
Iso 12 (13.30 kJ/mol)	**Iso 16 (18.49 kJ/mol)**
	

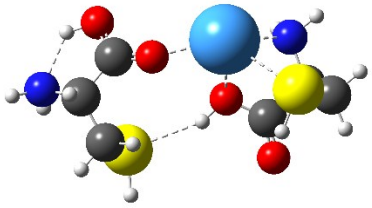
Conformations of Isomers 17-25 of $[(Cys)_2Na]^+$

Note: Energies include thermal correction at 298 K

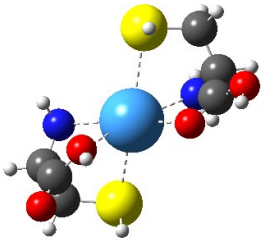
Iso 17 (18.87 kJ/mol)



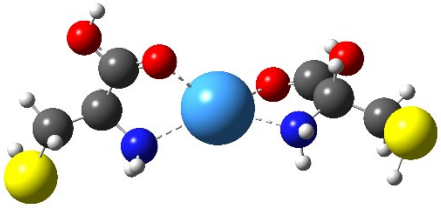
Iso 21 (21.26 kJ/mol)



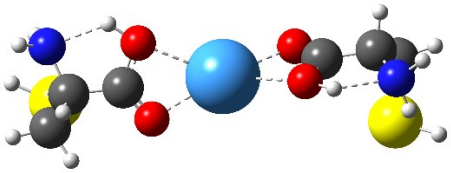
Iso 18 (19.78 kJ/mol)



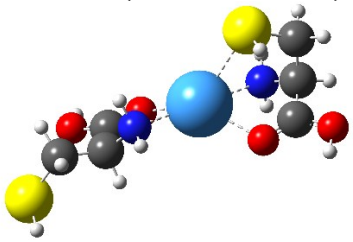
Iso 22 (21.51 kJ/mol)



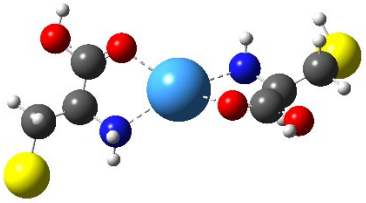
Iso 19 (20.72 kJ/mol)



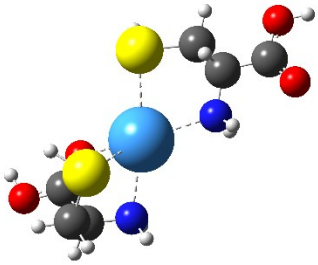
Iso 23 (22.09 kJ/mol)



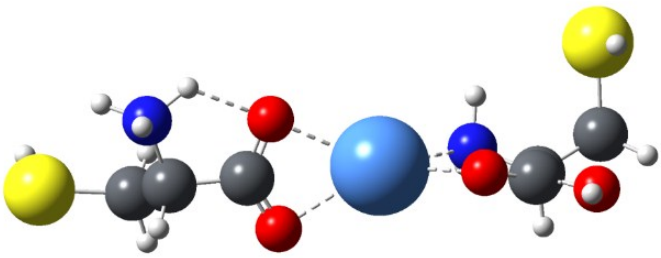
Iso 20 (21.07 kJ/mol)



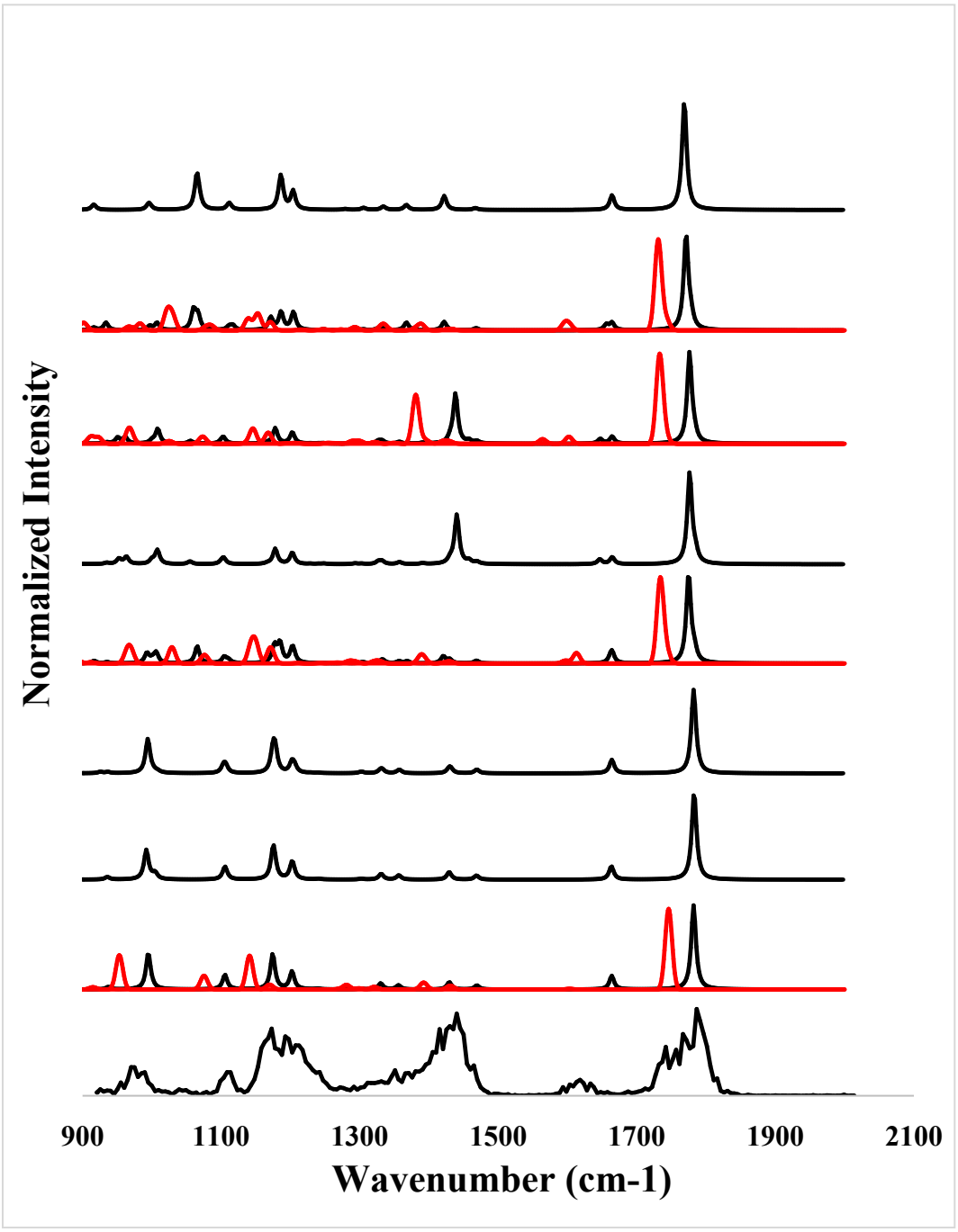
Iso 24 (22.29 kJ/mol)



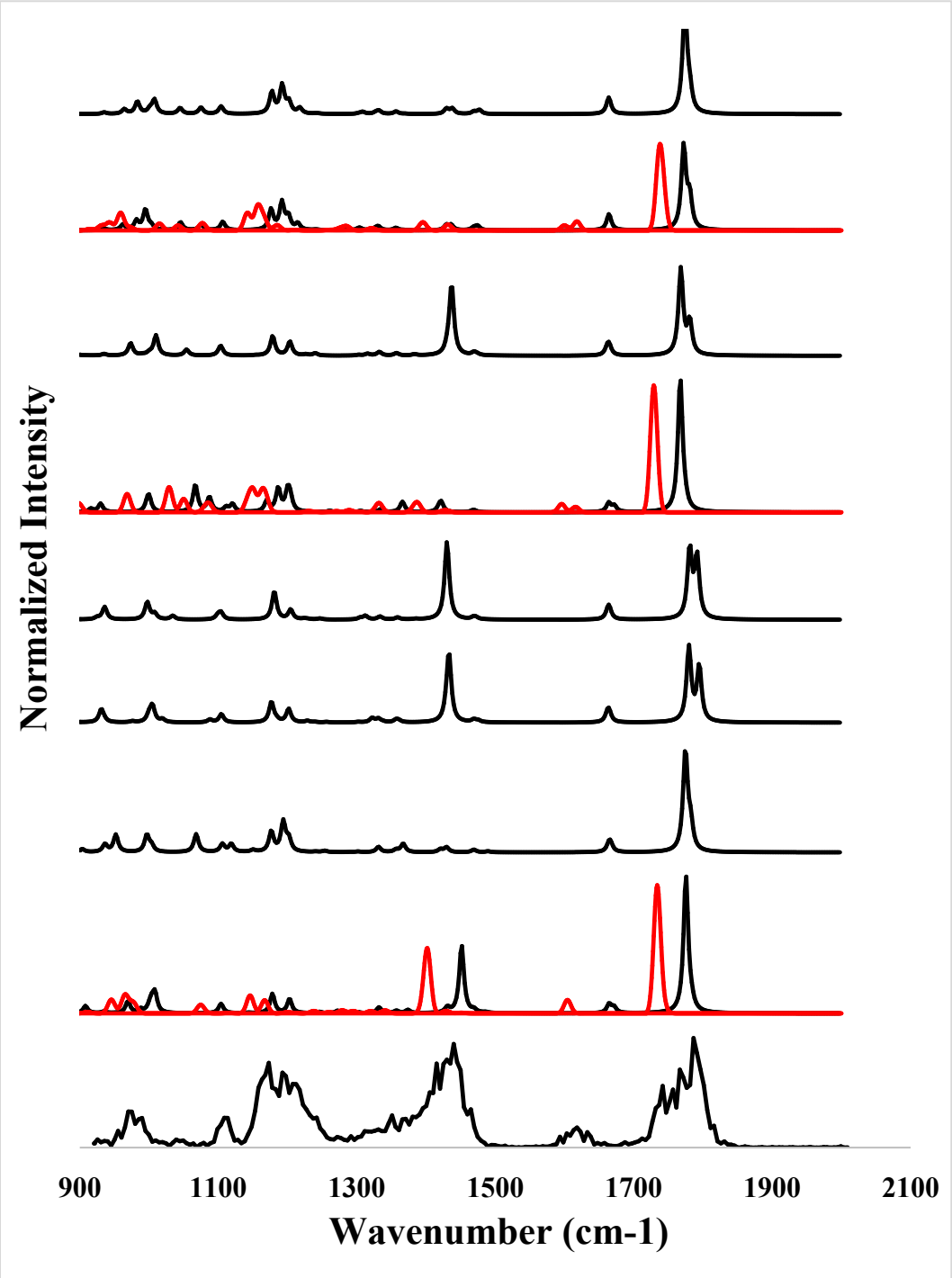
Iso 25 (ZW GM) (22.35 kJ/mol)



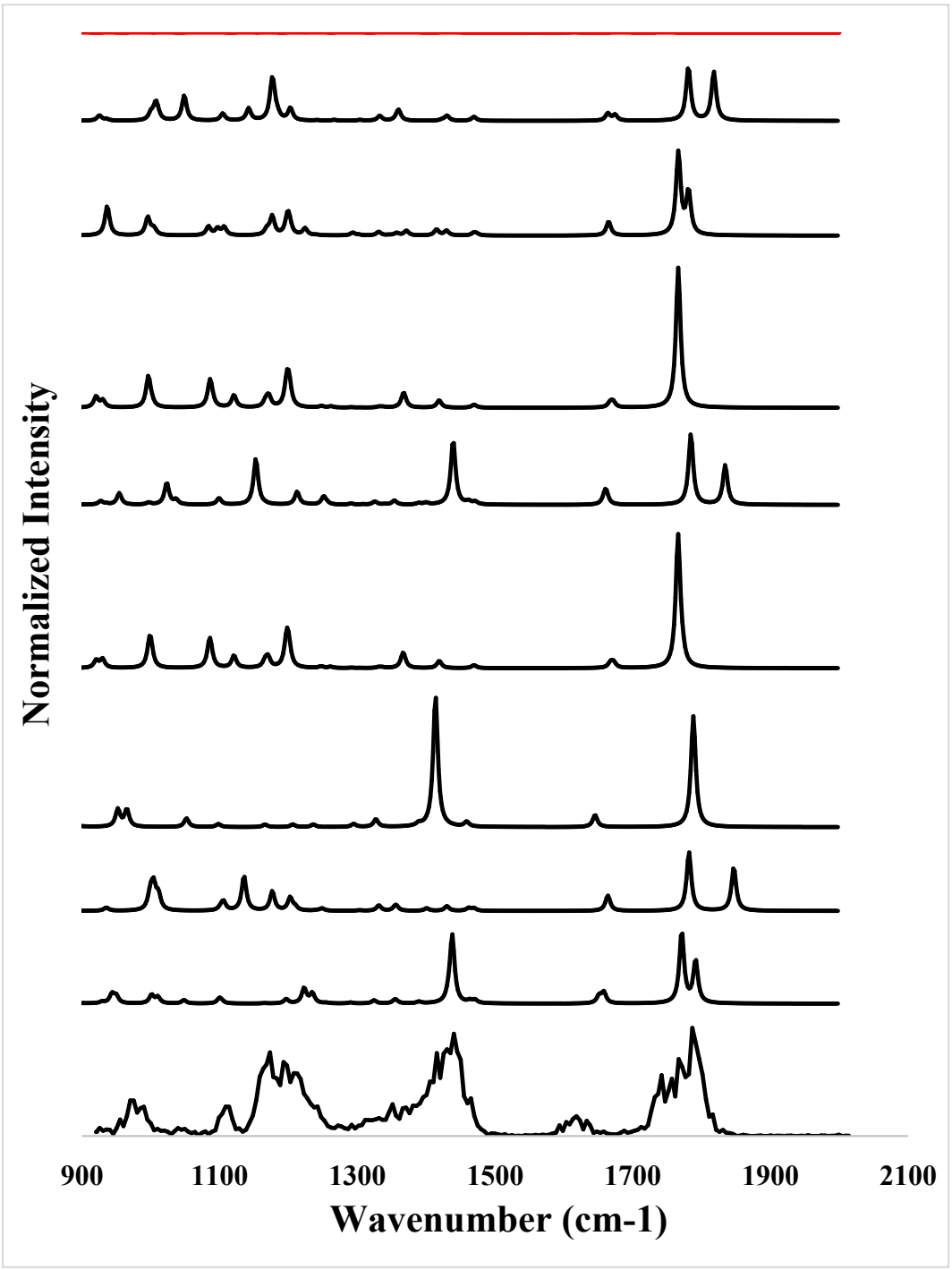
Predicted IR Spectra of Isomers 1-8 of $[(Cys)_2Na]^+$



Predicted IR Spectra of Isomers 9-16 of $[(Cys)_2Na]^+$

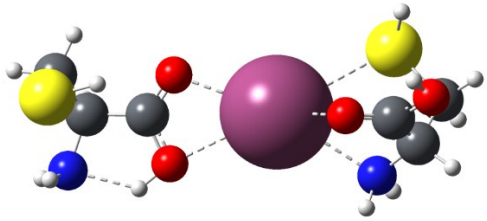
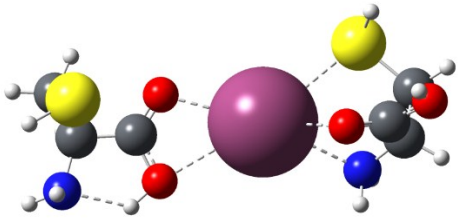
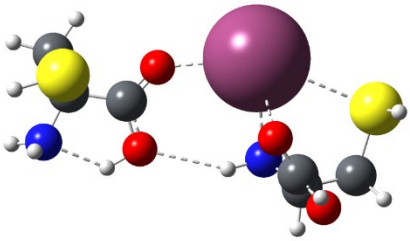
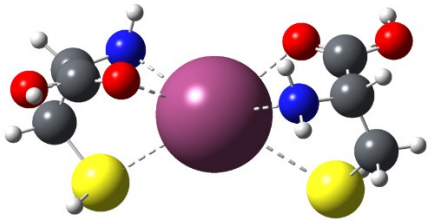
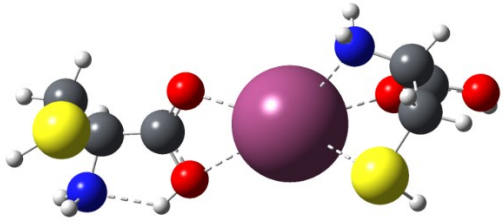
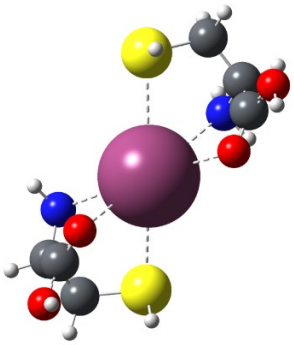
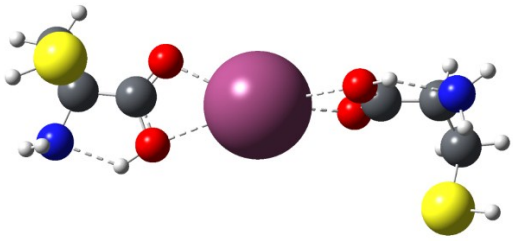
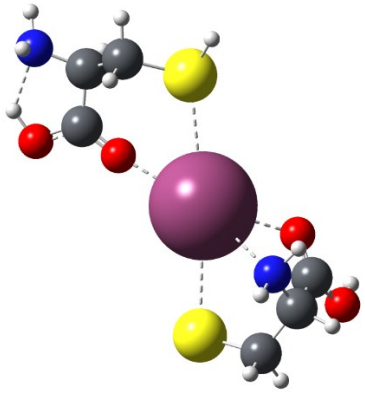


Predicted IR Spectra of Isomers 17-25 of $[(Cys)_2Na]^+$



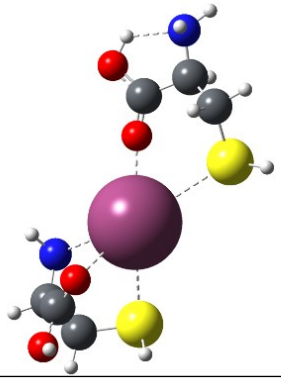
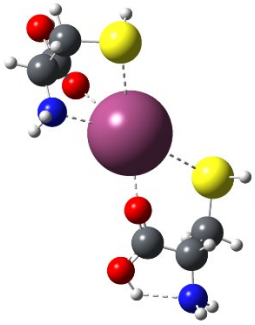
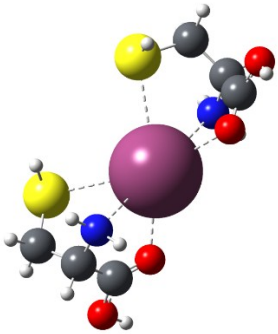
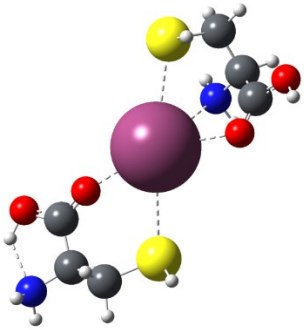
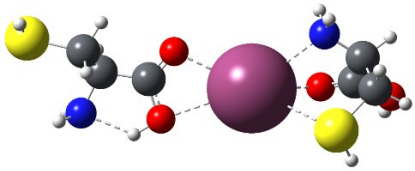
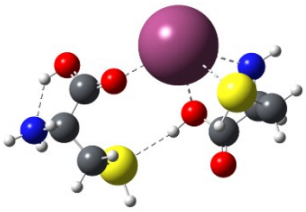
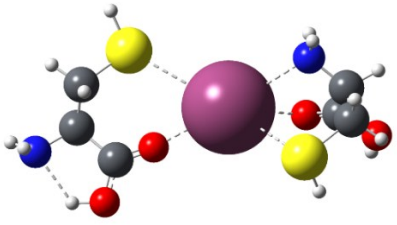
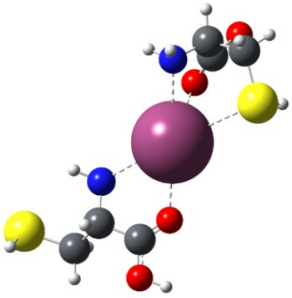
Conformations of Isomers 1-8 of $[(Cys)_2K]^+$

Note: Energies include thermal correction at 298 K

GM	**Iso 5 (2.14 kJ/mol)**
	
Iso 2 (0.57 kJ/mol)	**Iso 6 (3.90 kJ/mol)**
	
Iso 3 (1.20 kJ/mol)	**Iso 7 (4.37 kJ/mol)**
	
Iso 4 (2.06 kJ/mol)	**Iso 8 (7.04 kJ/mol)**
	

Conformations of Isomers 9-16 of $[(Cys)_2K]^+$

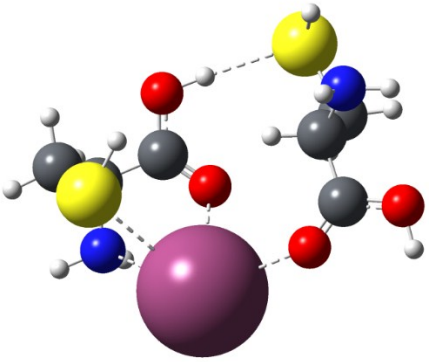
Note: Energies include thermal correction at 298 K

Iso 9 (8.06 kJ/mol)	**Iso 13 (11.41 kJ/mol)**
	
Iso 10 (8.12 kJ/mol)	**Iso 14 (12.28 kJ/mol)**
	
Iso 11 (8.38 kJ/mol)	**Iso 15 (12.43 kJ/mol)**
	
Iso 12 (9.37 kJ/mol)	**Iso 16 (12.93 kJ/mol)**
	

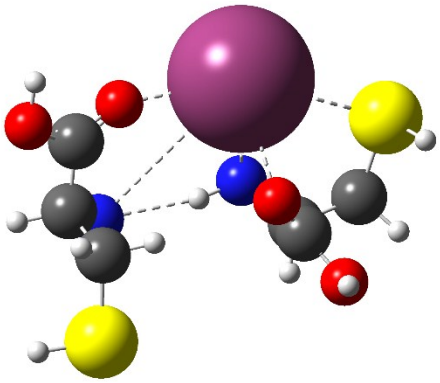
Conformations of Isomers 17-20 of $[(Cys)_2K]^+$

Note: Energies include thermal correction at 298 K

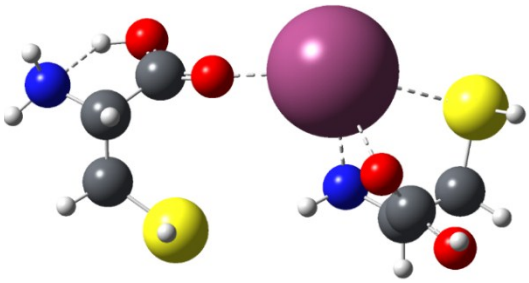
Iso 17 (14.06 kJ/mol)



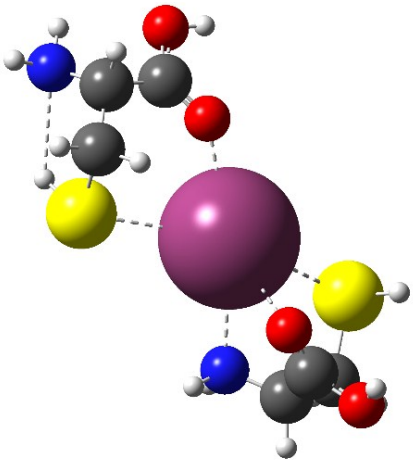
Iso 19 (17.67 kJ/mol)



Iso 18 (14.71 kJ/mol)

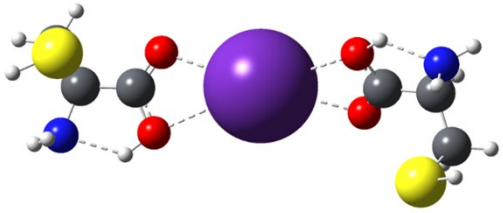
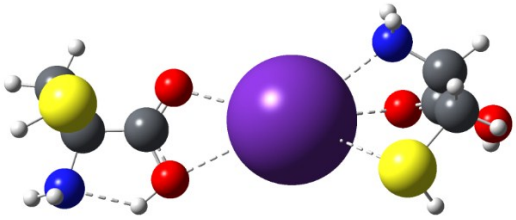
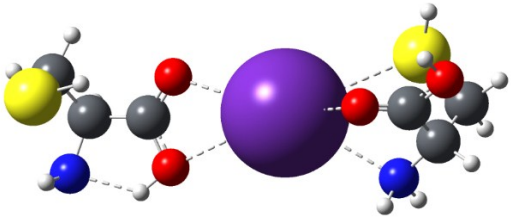
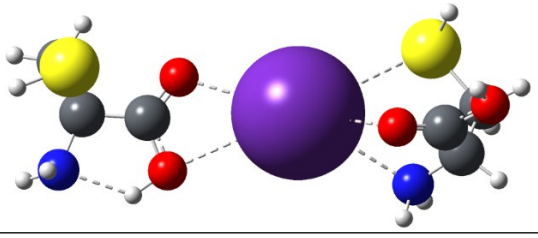
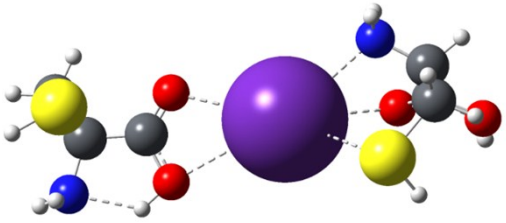
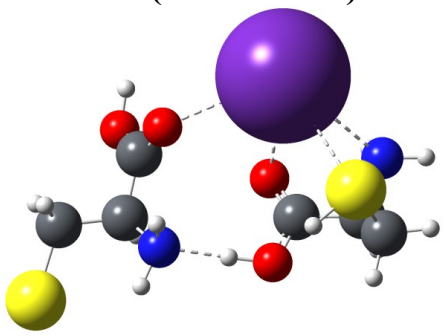
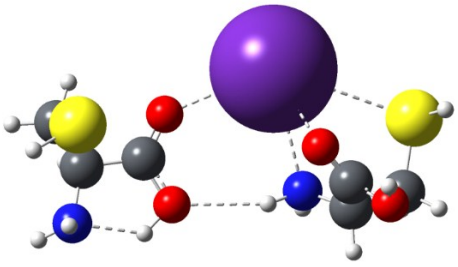
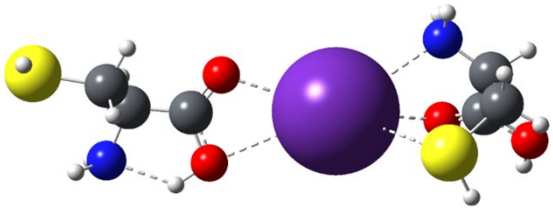


Iso 20 (19.17 kJ/mol)



Conformations of Isomers 1-8 of $[(Cys)_2Rb]^+$

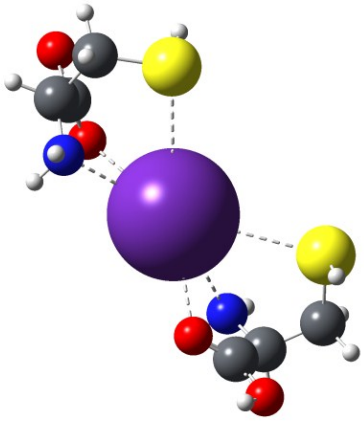
Note: Energies include thermal correction at 298 K

GM	**Iso 5 (5.61 kJ/mol)**
	
Iso 2 (3.98 kJ/mol)	**Iso 6 (6.10 kJ/mol)**
	
Iso 3 (5.61 kJ/mol)	**Iso 7 (8.81 kJ/mol)**
	
Iso 4 (5.61 kJ/mol)	**Iso 8 (12.82 kJ/mol)**
	

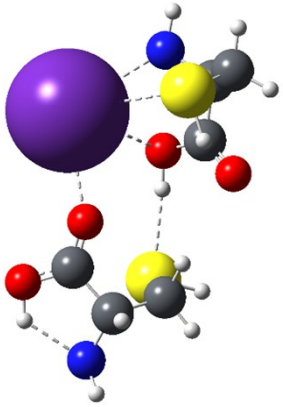
Conformations of Isomers 9-14 of $[(Cys)_2Rb]^+$

Note: Energies include thermal correction at 298 K

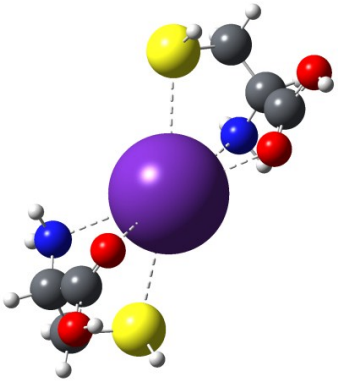
Iso 9 (12.84 kJ/mol)



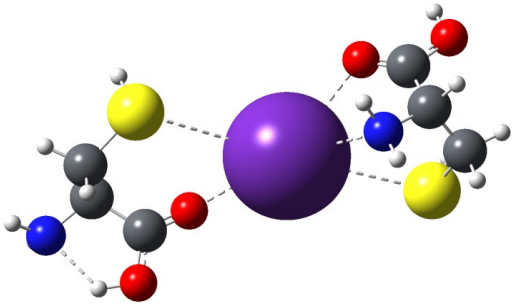
Iso 12 (14.33 kJ/mol)



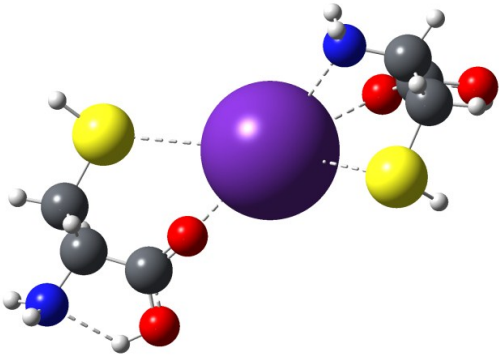
Iso 10 (13.01 kJ/mol)



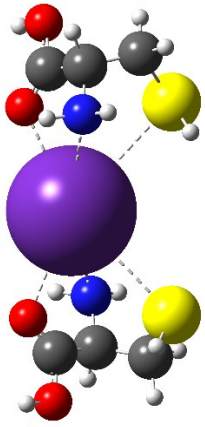
Iso 13 (15.23 kJ/mol)



Iso 11 (14.16 kJ/mol)

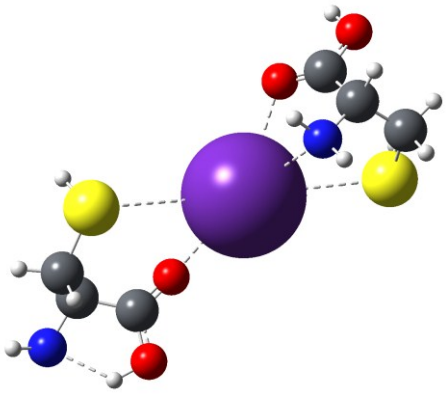
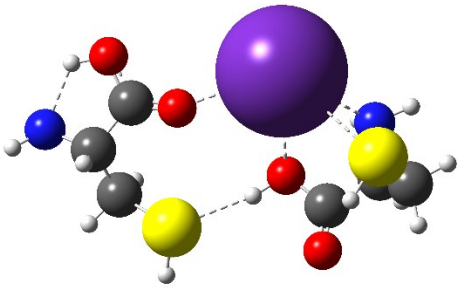
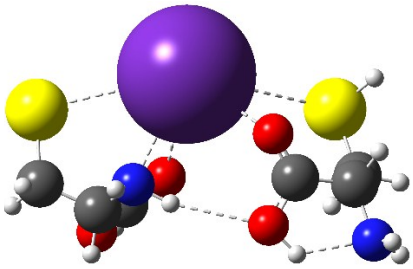
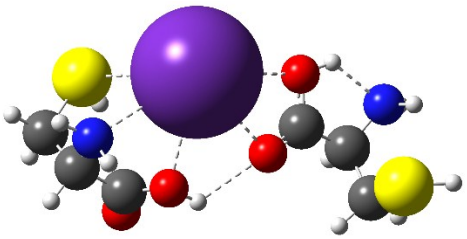
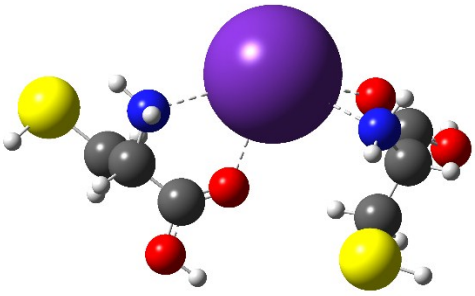
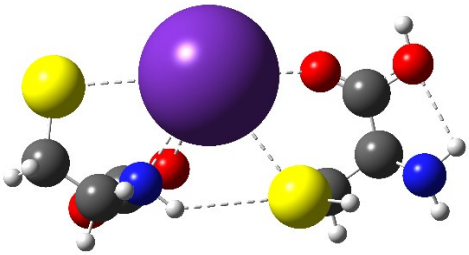


Iso 14 (16.80 kJ/mol)



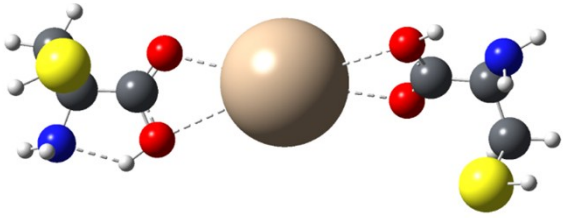
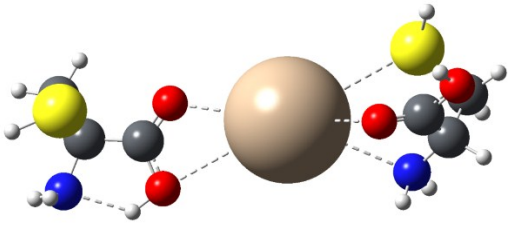
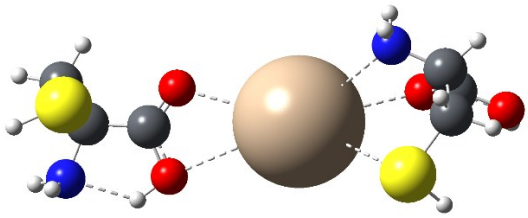
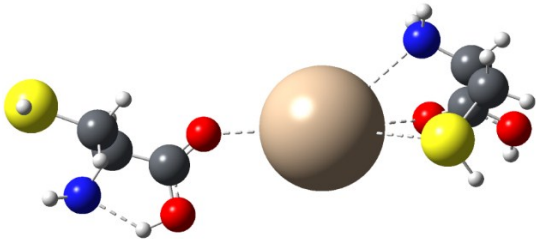
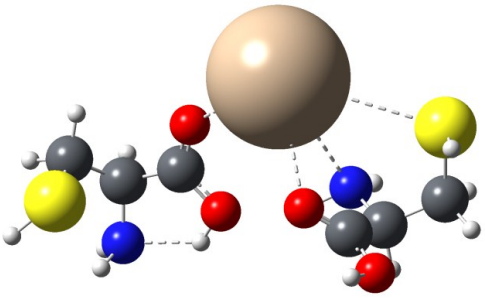
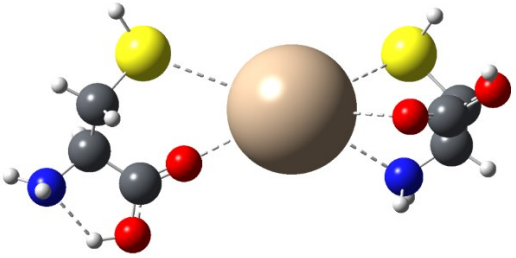
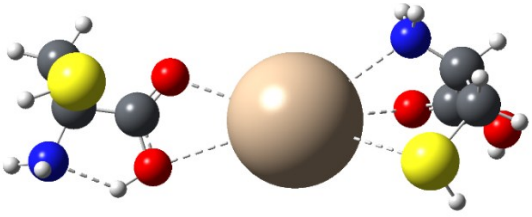
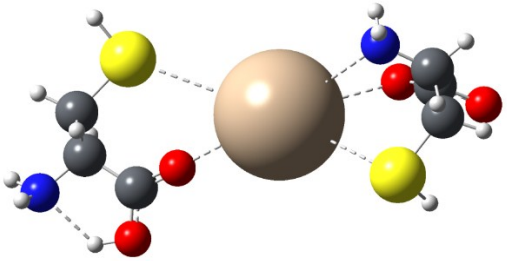
Conformations of Isomers 15-20 of $[(Cys)_2Rb]^+$

Note: Energies include thermal correction at 298 K

Iso 15 (17.69 kJ/mol)	**Iso 18 (22.94 kJ/mol)**
	
Iso 16 (18.40 kJ/mol)	**Iso 19 (23.99 kJ/mol)**
	
Iso 17 (22.54 kJ/mol)	**Iso 20 (25.16 kJ/mol)**
	

Conformations of Isomers 1-8 of $[(Cys)_2Cs]^+$

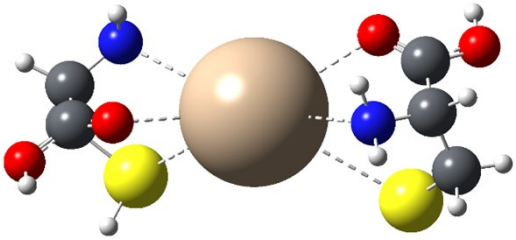
Note: Energies include thermal correction at 298 K

GM	**Iso 5 (10.19 kJ/mol)**
	
Iso 2 (7.36 kJ/mol)	**Iso 6 (16.83 kJ/mol)**
	
Iso 3 (8.26 kJ/mol)	**Iso 7 (18.42 kJ/mol)**
	
Iso 4 (9.83 kJ/mol)	**Iso 8 (18.84 kJ/mol)**
	

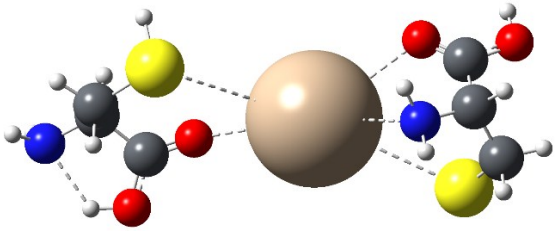
Conformations of Isomers 9-14 of $[(Cys)_2Cs]^+$

Note: Energies include thermal correction at 298 K

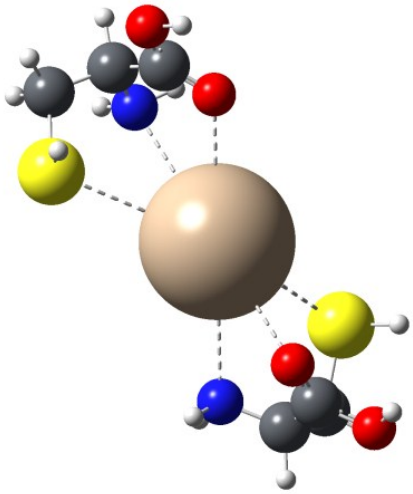
Iso 9 (20.63 kJ/mol)



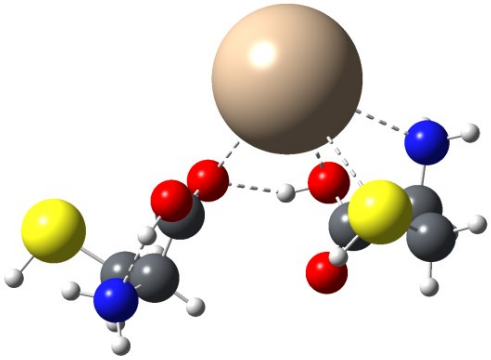
Iso 12 (22.70 kJ/mol)



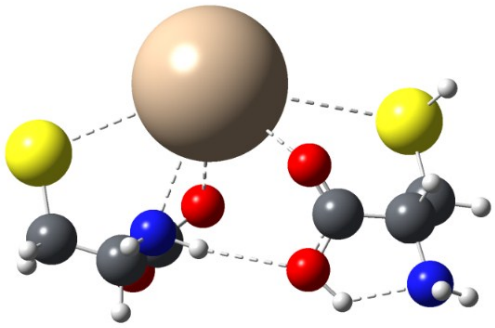
Iso 10 (20.81 kJ/mol)



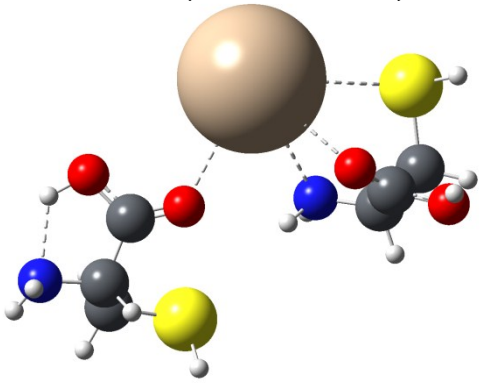
Iso 13 (22.88 kJ/mol)



Iso 11 (20.98 kJ/mol)



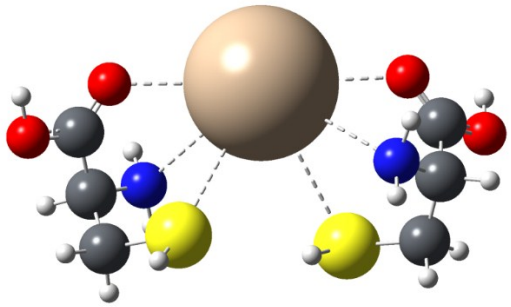
Iso 14 (24.56 kJ/mol)



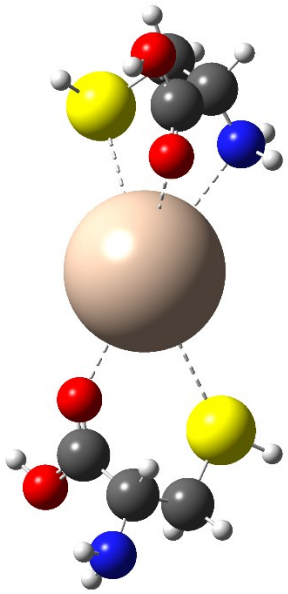
Conformations of Isomers 15-19 of $[(Cys)_2Cs]^+$

Note: Energies include thermal correction at 298 K

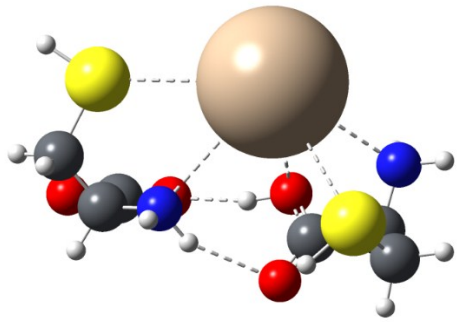
Iso 15 (24.92kJ/mol)



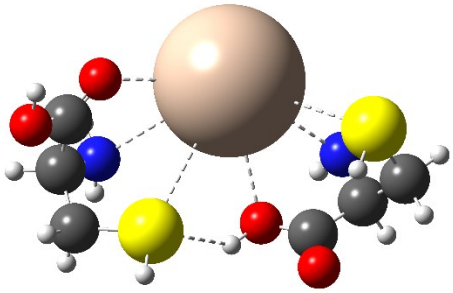
Iso 17 (36.74 kJ/mol)



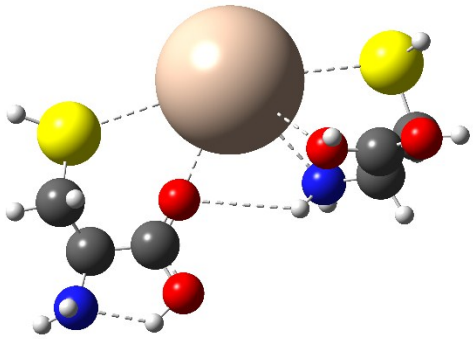
Iso 16 (27.88 kJ/mol)



Iso 18 (37.22 kJ/mol)



Iso 19 (38.58 kJ/mol)

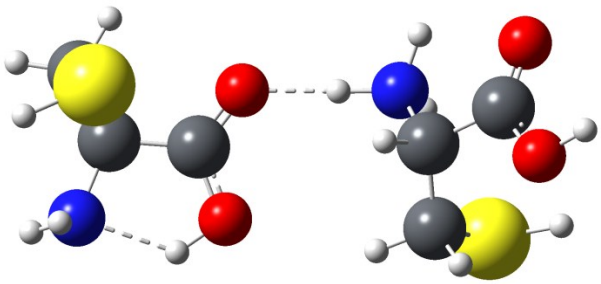


Atomic Coordinates $[(Cys)_2H]^+$

Note: Energies include thermal correction at 298 K

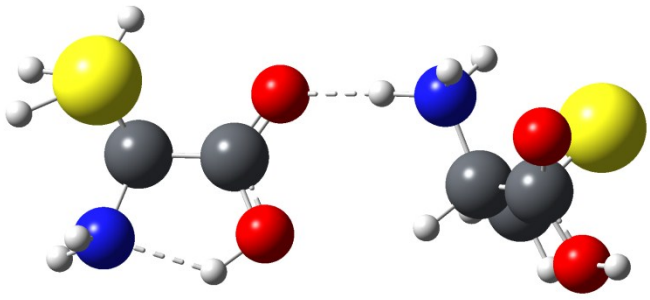
Iso_1 (GM)

H	-4.93250000	-1.48334300	-1.26354700
S	-3.76586500	-1.72845000	-0.63438900
C	-3.98621600	-0.53937700	0.75685500
H	-5.04882000	-0.42120900	0.96454400
H	-3.52208000	-1.00145600	1.62731300
C	-3.34033600	0.83212400	0.50573000
H	-3.52776100	1.45343000	1.39019800
N	-3.79126900	1.56866400	-0.67785700
H	-4.10666400	0.93956600	-1.41193000
H	-4.52729600	2.23434200	-0.47453100
C	-1.80881400	0.72155900	0.42440100
O	-1.14450100	0.02606500	1.17828600
O	-1.25354900	1.46672100	-0.51094400
H	-2.02920800	1.89865800	-0.97161600
H	4.50408900	1.39937200	-0.07075800
S	3.31431400	2.02149700	0.07044100
C	2.31112200	0.83512400	-0.90934900
H	1.35778900	1.33824500	-1.07743200
H	2.77281600	0.65056200	-1.87695900
C	2.05661400	-0.50544300	-0.20047100
H	1.28904600	-1.05729200	-0.75220400
N	1.54525500	-0.28665800	1.18883500
H	1.79620200	-1.09441700	1.77168800
H	2.03099200	0.53788500	1.57677400
C	3.27498100	-1.42642300	-0.08106100
O	3.56169900	-1.98983500	0.94365400
O	3.92285200	-1.53658400	-1.23869900
H	4.65540300	-2.16795900	-1.14093400
H	0.49880400	-0.12550000	1.20070500



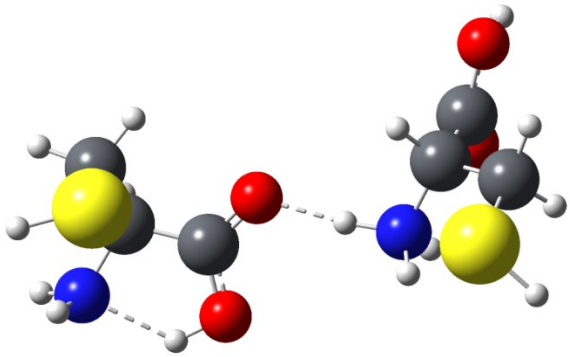
Iso_2 (6.40 kJ/mol)

H	-5.28791100	1.52569000	-0.07176500
S	-4.10669200	1.43249300	-0.71443300
C	-4.05227400	-0.40481800	-0.85202800
H	-5.06899200	-0.79449000	-0.87724500
H	-3.58279100	-0.62553900	-1.80991800
C	-3.25426700	-1.08360800	0.27248000
H	-3.28978300	-2.16602000	0.09727100
N	-3.69565400	-0.82535900	1.64571800
H	-4.13887300	0.08646300	1.72816600
H	-4.32914100	-1.53300600	1.99817300
C	-1.76145400	-0.72473100	0.19394500
O	-1.13446600	-0.66974800	-0.85277400
O	-1.18660500	-0.50963700	1.36299000
H	-1.93405400	-0.59518000	2.02230000
H	3.50710200	-2.74199100	-1.07181700
S	3.97561700	-1.50408500	-0.82160700
C	2.80380300	-1.10535300	0.55317800
H	2.07237500	-1.90747900	0.64068600
H	3.35396000	-1.03899000	1.48955000
C	2.08030700	0.22879300	0.31491400
H	1.29898500	0.34081800	1.07294000
N	1.41436600	0.25685500	-1.02527200
H	1.40561100	1.22769800	-1.36564700
H	1.99230300	-0.29355600	-1.68027100
C	2.96737000	1.47785900	0.38749400
O	2.90549400	2.35867600	-0.43177200
O	3.74878700	1.46526900	1.46281400
H	4.26963000	2.28525900	1.49515800
H	0.43120300	-0.13000200	-0.98402200



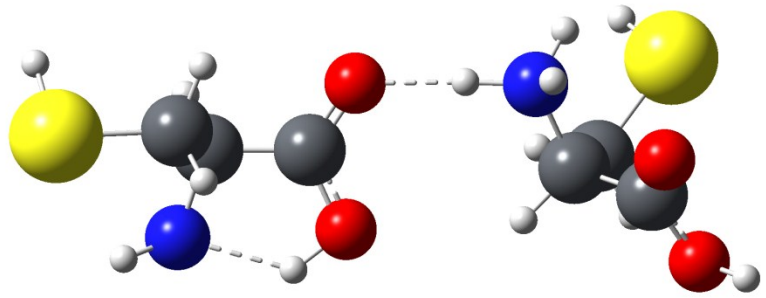
Iso_3 (7.43 kJ/mol)

H	-4.86948000	-1.72126600	1.14131100
S	-3.53287600	-1.55719800	1.19796100
C	-3.51991900	0.28527900	1.26215400
H	-2.70231900	0.56306400	1.92616800
H	-4.44975100	0.63554500	1.70811800
C	-3.30917000	0.94838000	-0.10801300
H	-3.32498100	2.03482800	0.04450100
N	-4.27509700	0.61959000	-1.15809100
H	-4.65337300	-0.31666800	-1.03647700
H	-5.04002200	1.28110100	-1.21532700
C	-1.90596800	0.65763000	-0.66484100
O	-0.89431700	0.66277300	0.02533600
O	-1.85956300	0.43608400	-1.95936300
H	-2.81270200	0.46666900	-2.25376200
H	3.92973100	-2.65059200	-1.49093800
S	3.12807900	-2.51574600	-0.41654000
C	3.68722700	-0.81920400	0.05684400
H	4.25870400	-0.87113100	0.98187900
H	4.33530300	-0.42720500	-0.72779900
C	2.48074600	0.11453700	0.28255100
H	1.89894600	-0.22275800	1.14172900
N	1.57091200	0.13174500	-0.90366400
H	1.88503400	0.85313200	-1.56363900
H	1.58913300	-0.79897000	-1.34494400
C	2.94771800	1.55395600	0.50380400
O	2.84929500	2.40293800	-0.34468400
O	3.49147100	1.70609400	1.70780500
H	3.81300200	2.61800100	1.80717400
H	0.56994400	0.35743800	-0.61619000



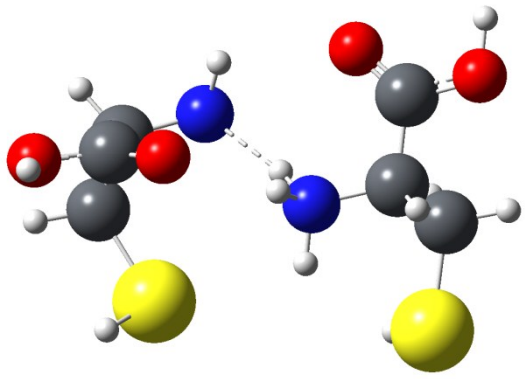
Iso_4 (9.69 kJ/mol)

H	5.79109900	-0.82816100	1.14721600
S	5.64045500	0.38429000	0.57359100
C	3.81086000	0.43042300	0.64254700
H	3.46583300	0.29778800	1.66656300
H	3.55229500	1.44555200	0.33017600
C	3.10997600	-0.59986900	-0.27412800
H	3.30080000	-1.60375000	0.11747600
N	3.49360000	-0.45008400	-1.68203700
H	4.39074800	0.02266700	-1.76406300
H	3.59282000	-1.34792100	-2.14518400
C	1.59857200	-0.35699800	-0.18029600
O	0.94055000	-0.57489500	0.82618000
O	1.05710300	0.14737600	-1.27511800
H	1.82193100	0.19130800	-1.92332400
H	-3.55116900	-2.98497300	0.47032400
S	-4.10126900	-1.75537800	0.47603300
C	-2.94684200	-0.99832000	-0.75526400
H	-2.15942000	-1.71323400	-0.98973000
H	-3.49021200	-0.77380000	-1.67082800
C	-2.32305600	0.30172200	-0.22493800
H	-1.54235900	0.62348600	-0.92129800
N	-1.67790100	0.09440900	1.10986100
H	-1.75907500	0.96749600	1.64855000
H	-2.21420700	-0.62894400	1.61502500
C	-3.29578200	1.47650700	-0.06034300
O	-3.30434200	2.16960600	0.92492000
O	-4.06263900	1.63567400	-1.13390900
H	-4.64007900	2.40763900	-1.00967800
H	-0.66361200	-0.19089400	1.01798100



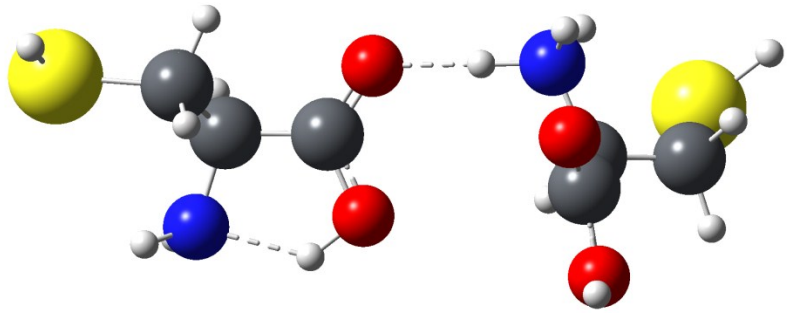
Iso_5 (12.01 kJ/mol)

H	2.77269600	2.08834800	0.98805900
S	2.04640600	2.09852500	-0.14786800
C	2.99459300	0.79397000	-1.04071100
H	2.91411500	1.04702100	-2.09957400
H	4.04495700	0.87475300	-0.76802900
C	2.50501100	-0.65392000	-0.83909100
H	3.21845700	-1.29718600	-1.37192700
N	1.13128200	-0.82429200	-1.33664700
H	1.09438300	-0.56219600	-2.31876800
H	0.84573300	-1.80104500	-1.29090200
C	2.57940800	-1.06096700	0.62941600
O	1.63051300	-1.29512300	1.34500800
O	3.84688800	-1.12097400	1.04471400
H	3.86540200	-1.38487200	1.97913600
H	-1.94410100	2.95522700	-0.64370800
S	-2.68290100	2.46615300	0.37188300
C	-2.94818000	0.78231700	-0.33494300
H	-4.01621200	0.57279100	-0.31622400
H	-2.62023900	0.77245300	-1.37472700
C	-2.22720800	-0.30747000	0.48457300
H	-2.63878100	-0.32334800	1.49613200
N	-0.77006400	-0.01976400	0.58851700
H	-0.64005000	0.96930600	0.83771500
H	-0.28099800	-0.59388300	1.28635900
C	-2.41481800	-1.68734600	-0.14475100
O	-1.53995100	-2.29652100	-0.70509000
O	-3.67623000	-2.09566500	-0.00430700
H	-3.78620300	-2.96309200	-0.42823300
H	-0.19635400	-0.21396500	-0.29220000



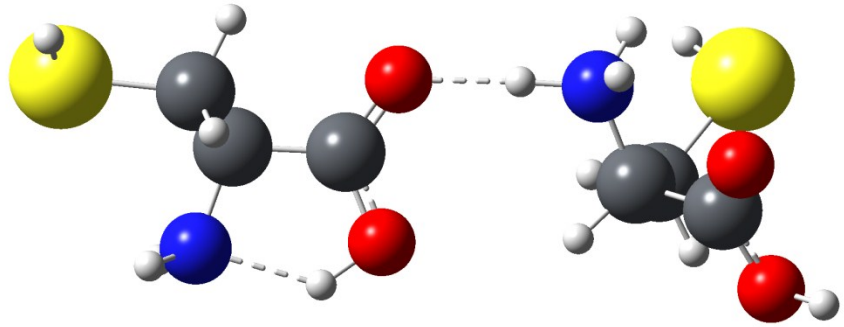
Iso_6 (13.33 kJ/mol)

H	5.05902600	-2.16821400	-0.78993800
S	4.06689000	-2.08114200	0.11735300
C	3.97621400	-0.23585700	0.16247600
H	4.37102000	0.12453000	1.11062900
H	4.58917500	0.16935200	-0.64349100
C	2.51675900	0.24243800	0.03054700
H	1.93133400	-0.07471300	0.89526200
N	1.86344500	-0.32192600	-1.19169900
H	2.26587500	-1.25179000	-1.37835400
H	2.02059400	0.31099400	-1.98520300
C	2.45278100	1.76480700	-0.09587500
O	2.19154100	2.31848900	-1.13324600
O	2.75342600	2.35845800	1.05560800
H	2.74094900	3.32302000	0.93683400
H	-5.85595100	0.84004000	-1.39283700
S	-5.45963900	-0.12778000	-0.54334500
C	-3.65569000	0.22991400	-0.67228700
H	-3.28704300	-0.03770500	-1.66104100
H	-3.48085700	1.29534000	-0.50276700
C	-2.90330200	-0.59893500	0.37973100
H	-3.08327000	-1.66114300	0.18308700
N	-3.24384500	-0.24955200	1.76787900
H	-3.98967000	0.43877500	1.81207300
H	-3.54805000	-1.05486300	2.30386300
C	-1.39132900	-0.38056300	0.20702500
O	-0.79018400	-0.63216200	-0.82745300
O	-0.78537300	0.10390300	1.27196900
H	-1.52775100	0.19450800	1.94498500
H	0.81350700	-0.42534600	-1.05521500



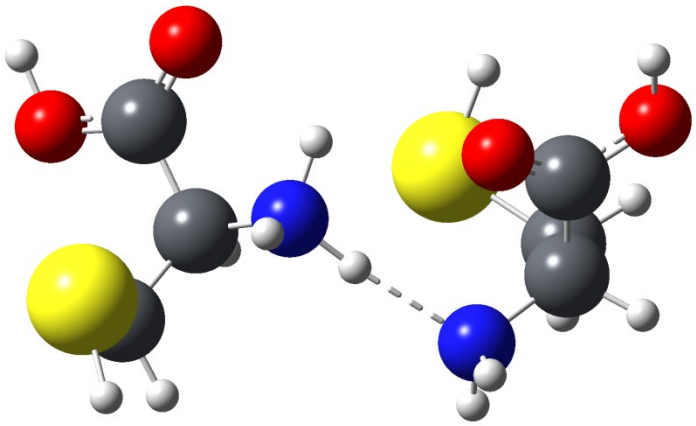
Iso_7 (13.54 kJ/mol)

H	6.04698600	-0.50720000	-1.68689400
S	5.64958900	0.17223000	-0.59332300
C	3.85403400	-0.20246900	-0.77582800
H	3.45356700	0.28858500	-1.66111300
H	3.71191100	-1.28198300	-0.87191600
C	3.10705100	0.31691900	0.46127200
H	3.25694000	1.39963400	0.53072500
N	3.48949300	-0.34578500	1.71839800
H	4.21433200	-1.04278800	1.57437700
H	3.83773600	0.30912700	2.40965300
C	1.59510600	0.10791800	0.27134100
O	0.96553300	0.56112800	-0.67310000
O	1.02141100	-0.60342900	1.22194500
H	1.78331400	-0.82533700	1.84150700
H	-3.37308200	3.09606000	0.14390100
S	-3.99489700	1.92899700	-0.11268700
C	-2.90425100	0.86879300	0.94016400
H	-2.07868500	1.47174300	1.31565600
H	-3.47215300	0.49689000	1.79050400
C	-2.35226900	-0.33216100	0.15689400
H	-1.60288900	-0.83704800	0.77453900
N	-1.67588100	0.10285200	-1.10560000
H	-1.79786300	-0.63633900	-1.81091800
H	-2.16232100	0.94394700	-1.45489700
C	-3.39154000	-1.38587500	-0.24650000
O	-3.42710300	-1.86210000	-1.35248100
O	-4.18285700	-1.71218600	0.77004200
H	-4.80416000	-2.40492700	0.48921200
H	-0.64862500	0.30448500	-0.95308000



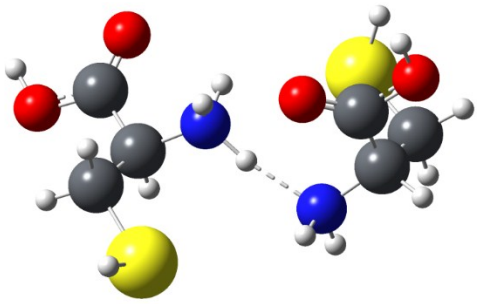
Iso_8 (16.92 kJ/mol)

H	-2.29488000	2.17831200	-0.47225500
S	-1.83828500	1.85792000	0.75562800
C	-3.11843200	0.59798000	1.16172100
H	-3.16939400	0.57973800	2.25230400
H	-4.08324900	0.94844000	0.80020700
C	-2.85664500	-0.82977100	0.64780200
H	-3.73916600	-1.42161200	0.92544800
N	-1.61807400	-1.39514400	1.21692600
H	-1.64584800	-1.30470600	2.23012200
H	-1.58591300	-2.39478800	1.02526000
C	-2.76673200	-0.87254600	-0.87522900
O	-1.77420600	-1.16743900	-1.49805400
O	-3.93125200	-0.53284500	-1.43688500
H	-3.84522900	-0.57942600	-2.40312600
H	3.45980200	-2.78630200	0.73996600
S	3.60297800	-1.68453200	-0.02142900
C	2.78813400	-0.50599800	1.15005300
H	2.33293100	-1.07240800	1.96180400
H	3.53730100	0.15893300	1.57476200
C	1.71964100	0.34345600	0.44596600
H	1.19050300	0.94101600	1.19366300
N	0.70935000	-0.50491000	-0.24825100
H	1.18170600	-1.34171600	-0.62037000
H	-0.10869000	-0.79582100	0.36030800
C	2.26077300	1.33411800	-0.59376400
O	1.75830300	1.47482800	-1.67836000
O	3.29936700	2.01961200	-0.12065900
H	3.59532800	2.66007800	-0.78885100
H	0.32265300	-0.00024200	-1.05479500



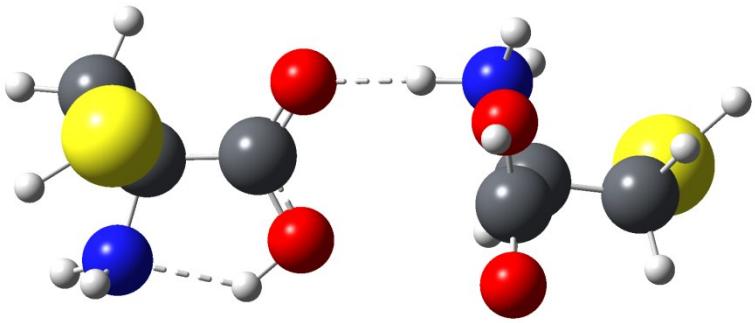
Iso_9 (17.08 kJ/mol)

H	2.60531900	3.41166300	0.37217000
S	2.13982900	2.52314700	-0.52682900
C	2.89316000	1.02648700	0.24984600
H	3.93919500	0.95088600	-0.03965500
H	2.83522100	1.10611900	1.33753700
C	2.16694500	-0.23278000	-0.22799900
H	2.17303300	-0.27015800	-1.32229900
N	0.73890700	-0.26478900	0.20992800
H	0.40698800	-1.23676000	0.25609500
H	0.59654200	0.13487000	1.14237200
C	2.81814000	-1.53332800	0.26510900
O	2.18919700	-2.41631000	0.78743500
O	4.12443500	-1.55293600	0.00900700
H	4.49807600	-2.40126500	0.30111400
H	-2.74563600	-2.33206700	0.42451700
S	-2.15449700	-2.02641900	-0.74839500
C	-3.14954300	-0.51902600	-1.11929700
H	-3.17869900	-0.45013000	-2.20848100
H	-4.17003800	-0.68345300	-0.77913800
C	-2.61708500	0.81029600	-0.54995600
H	-3.37422400	1.57034200	-0.78558700
N	-1.30219800	1.15519100	-1.11948100
H	-1.36362400	1.15847100	-2.13503700
H	-1.03707300	2.09985100	-0.84624600
C	-2.51086100	0.76552000	0.97172600
O	-1.47912500	0.83867500	1.59905500
O	-3.71526500	0.62798400	1.53333100
H	-3.61772800	0.61134000	2.49936400
H	0.05188800	0.26749800	-0.41347300



Iso_10 (17.98 kJ/mol)

H	-4.89506300	1.34275600	0.44217000
S	-3.77078100	1.37419200	-0.30074100
C	-3.81412900	-0.37472000	-0.88026900
H	-4.84895600	-0.70960600	-0.93732000
H	-3.40548300	-0.36932400	-1.89009600
C	-2.99440800	-1.33713700	-0.00658100
H	-3.08924800	-2.34024700	-0.44069900
N	-3.35394500	-1.41543500	1.41135800
H	-3.74658000	-0.53939500	1.74685000
H	-4.00095400	-2.16754100	1.61600600
C	-1.49246700	-1.02071700	-0.08304300
O	-0.91767300	-0.72357300	-1.12078800
O	-0.84841800	-1.12549600	1.06198300
H	-1.56000000	-1.34975400	1.72738700
H	5.15577800	-1.30173600	-1.01556300
S	4.20854600	-1.61569200	-0.11031800
C	3.71141700	0.11675000	0.29750900
H	3.98815700	0.33832300	1.32690800
H	4.24452400	0.80598400	-0.35816600
C	2.18593400	0.29266400	0.16392800
H	1.66964400	-0.34639400	0.88168800
N	1.71165000	-0.12188600	-1.19926500
H	1.86707400	0.62081300	-1.88544600
H	2.24833400	-0.96052200	-1.47072600
C	1.79864000	1.73638100	0.48109800
O	1.76801900	2.17164000	1.59304600
O	1.55720300	2.44261300	-0.64517400
H	1.34739400	3.36186100	-0.41100500
H	0.67425100	-0.36077600	-1.18808700

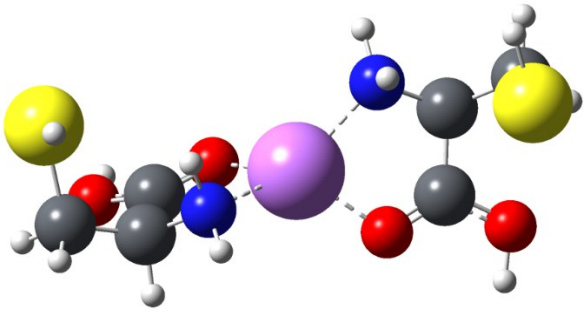


Atomic Coordinates $[(Cys)_2Li]^+$

Note: Energies include thermal correction at 298 K

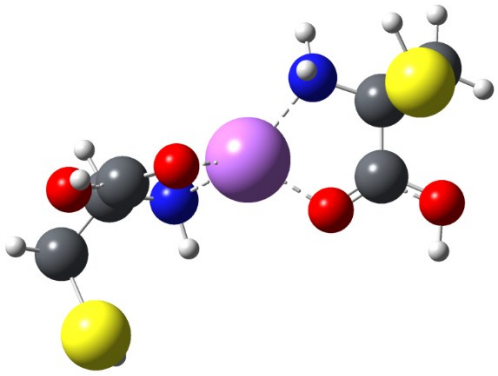
Iso_1 (GM)

H	4.12199300	-2.72864400	0.41603200
S	4.29225800	-1.66462500	-0.39327900
C	4.13867300	-0.35859900	0.90219100
H	4.30972600	-0.80775700	1.87970200
H	4.93237300	0.36460300	0.72301700
C	2.76903800	0.34672000	0.88872800
H	2.76938200	1.08042600	1.70521100
N	1.60494100	-0.53736300	1.07121500
H	1.80529900	-1.42481300	0.60685600
H	1.47348500	-0.74398100	2.05727900
C	2.53210600	1.17878300	-0.37352300
O	1.44635300	1.27468700	-0.91616900
O	3.61182400	1.82502700	-0.79041800
H	3.38802800	2.36415700	-1.56705300
H	-4.12163700	-2.72860000	-0.41588400
S	-4.29230100	-1.66456900	0.39332700
C	-4.13872500	-0.35857800	-0.90218100
H	-4.30977600	-0.80777100	-1.87967700
H	-4.93243100	0.36462300	-0.72303200
C	-2.76909300	0.34672800	-0.88873200
H	-2.76942700	1.08043900	-1.70521300
N	-1.60500700	-0.53736100	-1.07126900
H	-1.80530000	-1.42474700	-0.60676100
H	-1.47370900	-0.74412000	-2.05732500
C	-2.53207500	1.17878300	0.37351900
O	-1.44621800	1.27486100	0.91592000
O	-3.61177600	1.82491200	0.79063600
H	-3.38788400	2.36409000	1.56721200
Li	0.00000600	0.32778100	-0.00017600



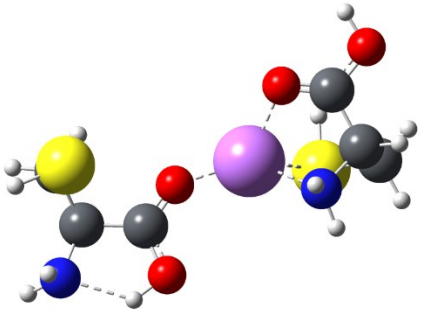
Iso_2 (1.27 kJ/mol)

H	-4.31393600	2.33471500	-0.36141500
S	-4.25422100	1.13952900	-0.98167500
C	-4.28160300	0.08827500	0.53338800
H	-4.73611000	0.64931000	1.34926000
H	-4.92543200	-0.76220300	0.31506600
C	-2.88484600	-0.40532500	0.95684700
H	-3.01141100	-1.00858900	1.86528700
N	-1.90250300	0.65264700	1.24747700
H	-2.05034200	1.41947700	0.58850500
H	-2.06183900	1.03156700	2.17636000
C	-2.25408000	-1.36176500	-0.05700300
O	-1.06605000	-1.36508900	-0.32363900
O	-3.11774400	-2.22007900	-0.58056000
H	-2.65406500	-2.81438400	-1.19355300
H	4.31400200	-2.33471600	-0.36139700
S	4.25424300	-1.13953700	-0.98166500
C	4.28161000	-0.08827300	0.53339100
H	4.73611000	-0.64930200	1.34927100
H	4.92544300	0.76220300	0.31506900
C	2.88484900	0.40533000	0.95683600
H	3.01140200	1.00860000	1.86527500
N	1.90249700	-0.65263400	1.24745700
H	2.05034100	-1.41946900	0.58849000
H	2.06181400	-1.03154800	2.17634500
C	2.25407700	1.36174300	-0.05702900
O	1.06603700	1.36506200	-0.32361800
O	3.11770400	2.22012600	-0.58053500
H	2.65399900	2.81444700	-1.19349300
Li	0.00003100	-0.00004900	0.57935900



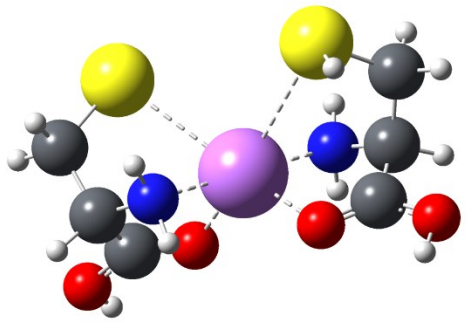
Iso_3 (2.74 kJ/mol)

H	-5.15055900	1.83266200	0.38278500
S	-3.80928500	1.86840200	0.25385900
C	-3.66489700	0.61874900	-1.09391900
H	-4.57907900	0.62352200	-1.68595800
H	-2.84820400	0.95286500	-1.73255200
C	-3.36831800	-0.80279700	-0.59080200
H	-3.31738100	-1.45885400	-1.46880700
N	-4.32333200	-1.38069100	0.35664800
H	-4.76562400	-0.66224300	0.92448100
H	-5.04126700	-1.93644800	-0.09230800
C	-1.96886000	-0.89636000	0.04182500
O	-0.98601000	-0.34537700	-0.43341300
O	-1.89754600	-1.64732900	1.11527100
H	-2.83573400	-1.94275500	1.27732200
H	3.22051900	-1.01872300	-2.04820700
S	2.81913700	-1.73212600	-0.97609900
C	3.93944200	-0.94616300	0.26469300
H	4.15239300	-1.72357200	1.00051500
H	4.88201400	-0.68287800	-0.21227000
C	3.33509800	0.27428700	0.99611400
H	4.07871300	0.62656100	1.71940600
N	2.04363500	-0.09280700	1.60171200
H	1.73381800	0.62807800	2.24995900
H	2.13759300	-0.94477400	2.14891400
C	3.06027500	1.38874200	-0.00552900
O	1.98603200	1.51622400	-0.56291000
O	4.11501200	2.15677400	-0.23916600
H	3.89342500	2.82141800	-0.91317800
Li	0.83442900	-0.08062300	-0.13844600



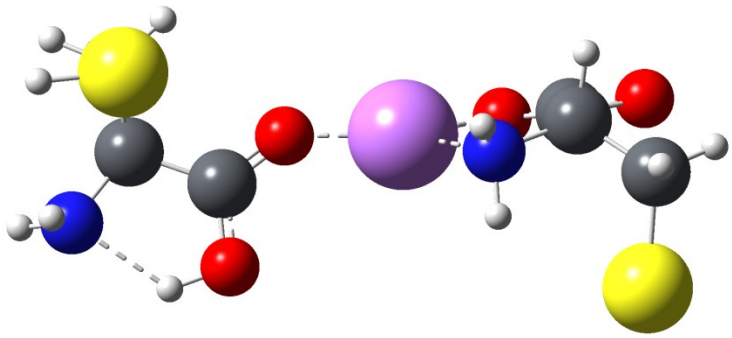
Iso_4 (4.12 kJ/mol)

H	-2.63734585	-1.48471159	1.82396228
S	-2.14316716	-1.94332120	0.65593627
C	-3.27367051	-0.99642431	-0.44980498
H	-3.41193374	-1.61854110	-1.33611371
H	-4.24609182	-0.89349239	0.02848388
C	-2.74671099	0.38464164	-0.89731190
H	-3.52277343	0.83625810	-1.52680828
N	-1.44893101	0.24922154	-1.57474530
H	-1.48948069	-0.49607749	-2.26456561
H	-1.21979053	1.09986492	-2.08427046
C	-2.53885493	1.28164717	0.31477631
O	-1.45211613	1.46859575	0.82574847
O	-3.67400511	1.79787896	0.77483389
H	-3.49138554	2.33450283	1.56365103
H	2.64235045	-1.48460663	-1.82376305
S	2.14450947	-1.94236883	-0.65696406
C	3.27286967	-0.99613354	0.45168215
H	3.40871360	-1.61841539	1.33823887
H	4.24645501	-0.89354328	-0.02429742
C	2.74516579	0.38504644	0.89804460
H	3.51958081	0.83636883	1.52977263
N	1.44539303	0.24964293	1.57158971
H	1.48378936	-0.49556288	2.26161802
H	1.21421314	1.10035560	2.08004924
C	2.54099803	1.28205757	-0.31467730
O	1.45596654	1.46804743	-0.82970644
O	3.67729767	1.79943410	-0.77050243
H	3.49706192	2.33584752	-1.56001876
Li	0.00173595	0.24973131	-0.00448367



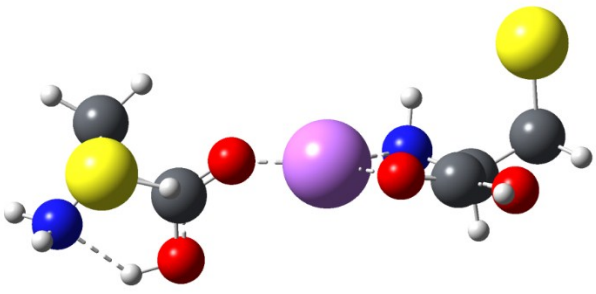
Iso_5 (5.54 kJ/mol)

H	5.42185200	-0.11477500	1.94059500
S	4.11668600	-0.42886500	1.82053400
C	4.18041600	-1.07136100	0.09362700
H	5.17693200	-1.46236900	-0.10700100
H	3.47865000	-1.90336200	0.05112100
C	3.79910000	-0.02852800	-0.96846100
H	3.86910100	-0.51625200	-1.94897400
N	4.59896400	1.19657500	-1.00980500
H	4.95878600	1.43972100	-0.09028500
H	5.36989600	1.14616900	-1.66478300
C	2.32262500	0.38608800	-0.85016800
O	1.42191100	-0.41087100	-0.61800700
O	2.08735100	1.65764400	-1.05536300
H	2.98832700	2.06156300	-1.19626800
H	-4.72339700	1.31999900	-0.95945300
S	-4.36635900	1.78419000	0.25614500
C	-4.31389300	0.15724200	1.11018500
H	-4.34234500	0.39559400	2.17453600
H	-5.20782900	-0.41695300	0.87388700
C	-3.04002400	-0.66162700	0.82131700
H	-3.06892800	-1.55204400	1.46265000
N	-1.77606500	0.05321500	1.07959900
H	-1.92779700	1.04662000	0.88813700
H	-1.52748900	-0.01667300	2.06225000
C	-2.98424700	-1.21516600	-0.60216800
O	-1.96285200	-1.25096200	-1.26695600
O	-4.14263100	-1.69333100	-1.03086400
H	-4.02940100	-2.07695900	-1.91678200
Li	-0.40531800	-0.53458500	-0.38051000



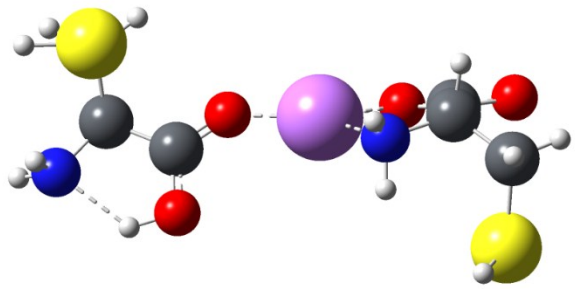
Iso_6 (8.22 kJ/mol)

H	3.15229500	2.05487300	-0.15423600
S	4.38765600	1.82355400	0.33644700
C	3.95602600	0.34444000	1.33909500
H	4.80550600	0.20301100	2.00840400
H	3.07841200	0.55269700	1.94899300
C	3.74668900	-0.94096300	0.51893900
H	3.63237900	-1.76879700	1.22950900
N	4.81016500	-1.27761000	-0.43000100
H	5.31834200	-0.44410900	-0.72028300
H	5.46692500	-1.95718400	-0.06570000
C	2.42235700	-0.91634400	-0.26215500
O	1.36372900	-0.53644900	0.22643600
O	2.50143300	-1.36276700	-1.48893900
H	3.47255200	-1.57947500	-1.60761900
H	-4.90530300	-1.36966600	2.03324400
S	-4.77138500	-0.12218200	1.54151700
C	-4.66708400	-0.58460500	-0.24250400
H	-5.04542100	-1.59805400	-0.36977000
H	-5.32369300	0.08881400	-0.79069400
C	-3.23447500	-0.49332200	-0.80237200
H	-3.26938100	-0.81466700	-1.85130700
N	-2.23459600	-1.32138800	-0.10194300
H	-2.48820000	-1.35126200	0.88813900
H	-2.27271300	-2.27858700	-0.44080800
C	-2.69879000	0.93895200	-0.85659800
O	-1.53954100	1.22635900	-0.61003900
O	-3.59884800	1.82735800	-1.24325100
H	-3.19053300	2.70802000	-1.29293800
Li	-0.42767400	-0.26651100	-0.12627700



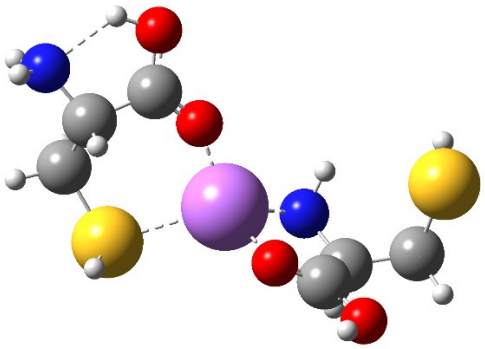
Iso_7 (9.57 kJ/mol)

H	5.53313100	-0.53861500	1.76378100
S	4.22104300	-0.81809800	1.63399900
C	4.20368600	-1.05011100	-0.19495600
H	5.18789900	-1.38092800	-0.52365100
H	3.49550800	-1.85326000	-0.39480600
C	3.78215600	0.20591100	-0.97337600
H	3.80985700	-0.04396500	-2.04151700
N	4.58372300	1.41289700	-0.76542900
H	4.98443000	1.43905800	0.16887100
H	5.32500100	1.52019700	-1.44725300
C	2.31309700	0.57303800	-0.70339800
O	1.41989200	-0.26134500	-0.62689900
O	2.07441300	1.85650000	-0.59944300
H	2.97096700	2.28643500	-0.67990100
H	-4.18545400	2.41408400	1.29841800
S	-4.49951300	1.63950100	0.24121100
C	-4.35616700	0.00982900	1.09484200
H	-4.42582300	0.16378000	2.17094400
H	-5.21120800	-0.58979400	0.78719300
C	-3.04746300	-0.73165300	0.76124300
H	-3.04575300	-1.66969800	1.33126700
N	-1.81000900	0.00233600	1.08364900
H	-1.98061000	0.99839600	0.92967600
H	-1.58223400	-0.10499000	2.06797600
C	-2.96063800	-1.17001500	-0.70223100
O	-1.92628600	-1.13837600	-1.34724700
O	-4.10166900	-1.63211200	-1.18614200
H	-3.97303400	-1.92576400	-2.10372300
Li	-0.40066300	-0.46111500	-0.39102100



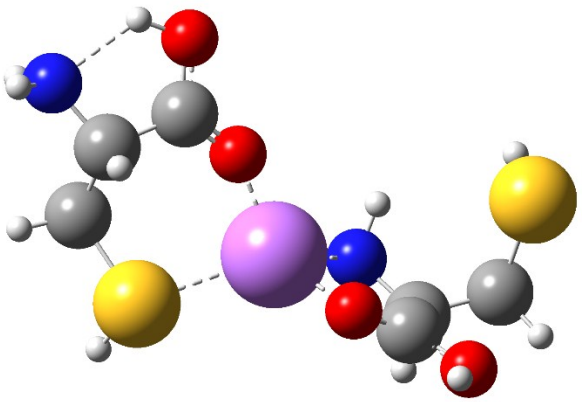
Iso_8 (9.73 kJ/mol)

H	2.29652500	-2.61416500	-0.64963800
S	2.12450800	-2.07096600	0.57371700
C	3.57559000	-0.93573100	0.53683200
H	3.66178100	-0.56710800	1.56184100
H	4.45600500	-1.54524200	0.33382400
C	3.55161600	0.24160300	-0.46231400
H	3.29992000	-0.14010600	-1.45666300
N	4.84419000	0.93326100	-0.54726000
H	5.41498500	0.81694800	0.28453200
H	5.39251500	0.65438200	-1.35206500
C	2.46477100	1.29298000	-0.13742300
O	1.30479500	1.00491500	0.10542300
O	2.87631000	2.53635400	-0.16057700
H	3.84095300	2.49275400	-0.38534000
H	-3.72602000	2.48595300	0.97064400
S	-3.96759600	1.73776800	-0.12441500
C	-4.07237300	0.10492600	0.72398200
H	-4.39161600	0.25470600	1.75495500
H	-4.85116000	-0.45981200	0.21371900
C	-2.74979100	-0.68469700	0.69853100
H	-2.92548600	-1.63776900	1.21441300
N	-1.60460200	-0.02458700	1.34524400
H	-1.65198200	0.97862800	1.15902700
H	-1.65455700	-0.13864500	2.35316000
C	-2.32030500	-1.08260200	-0.71460900
O	-1.16129800	-1.07295300	-1.09057000
O	-3.32563400	-1.48706800	-1.47722900
H	-2.98704800	-1.74941700	-2.34913400
Li	0.12901700	-0.44317500	0.22854400



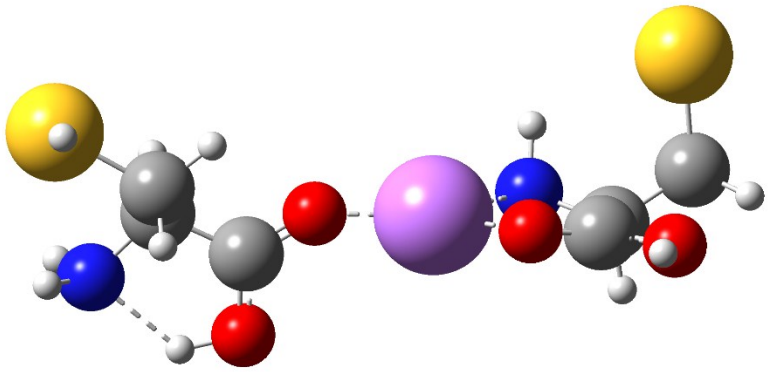
Iso 9 (13.92 kJ/mol)

H	2.36631000	2.90194500	-1.29647300
S	2.19500000	2.08368800	-0.23858000
C	3.54309500	0.88832800	-0.66637100
H	3.38389100	0.49842700	-1.67355200
H	4.48206900	1.43997900	-0.64169800
C	3.63471200	-0.26149600	0.35574900
H	3.56028000	0.15638200	1.36623000
N	4.88411200	-1.02448800	0.27857900
H	5.28532600	-1.03764200	-0.65441400
H	5.58987500	-0.69204000	0.92500500
C	2.45775500	-1.25563700	0.23934100
O	1.30265200	-0.90452800	0.06676800
O	2.78640100	-2.51768400	0.36228700
H	3.77135800	-2.52865400	0.46783300
H	-3.65702400	-2.56620900	-0.89892400
S	-3.93281400	-1.76952000	0.15294800
C	-4.06307400	-0.18522800	-0.77997400
H	-4.35404100	-0.39650900	-1.80855300
H	-4.86865900	0.38247700	-0.31675300
C	-2.76391000	0.64266700	-0.76578200
H	-2.95236600	1.56004600	-1.33857400
N	-1.58374800	-0.01902800	-1.34619800
H	-1.60588900	-1.00920500	-1.09531900
H	-1.61867700	0.02678000	-2.36016000
C	-2.38125400	1.12955600	0.63274300
O	-1.23245900	1.17288200	1.03430900
O	-3.41582700	1.54628500	1.34841000
H	-3.10478700	1.86720700	2.21109900
Li	0.11157800	0.51671700	-0.21024200



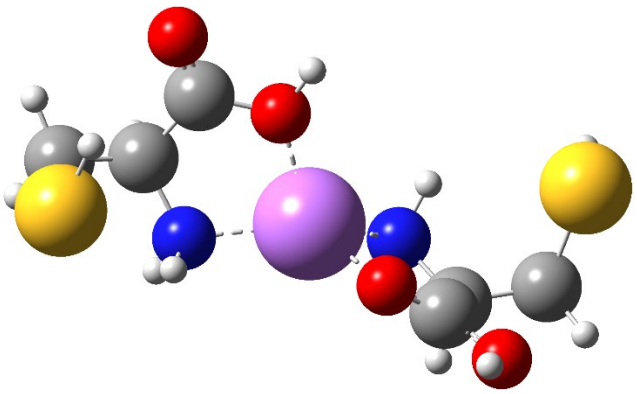
Iso 10 (15.98 kJ/mol)

H	5.58148900	2.30481800	-1.28331200
S	5.43208600	1.70370200	-0.08682400
C	3.88254300	0.79985000	-0.51500000
H	3.04062600	1.48943400	-0.54182700
H	3.99401200	0.33308600	-1.49648900
C	3.61338500	-0.27774400	0.54836400
H	3.50086100	0.21009100	1.52259600
N	4.63766700	-1.33036200	0.57539000
H	5.45167200	-1.07767500	0.02261300
H	4.96299300	-1.52728400	1.51563400
C	2.26529900	-0.95019200	0.23786100
O	1.20099900	-0.34344200	0.25183000
O	2.34189900	-2.22327000	-0.05139600
H	3.31918700	-2.43297900	0.03186200
H	-4.77362000	1.28751400	2.36039700
S	-4.74989900	1.47449000	1.02604100
C	-4.82704400	-0.30441700	0.53965400
H	-5.18075700	-0.88985300	1.38735100
H	-5.56420000	-0.39015300	-0.25685300
C	-3.46977300	-0.85476500	0.06109900
H	-3.60970500	-1.91757100	-0.17475200
N	-2.36906800	-0.74257000	1.03644800
H	-2.50791700	0.11741200	1.57167600
H	-2.41047100	-1.50918900	1.70204400
C	-2.99498000	-0.22870200	-1.25184700
O	-1.82684800	0.03715500	-1.47910600
O	-3.96368700	-0.04887400	-2.13430300
H	-3.59469900	0.31572800	-2.95626400
Li	-0.61338100	-0.37688000	-0.04400400



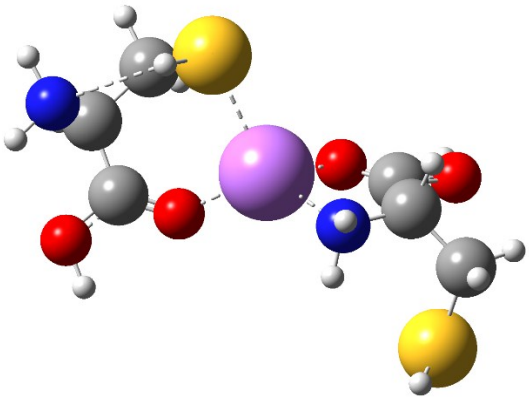
Iso 11 (20.75 kJ/mol)

H	-4.54384900	2.28737800	0.29516000
S	-4.34695800	1.28295700	-0.58131300
C	-4.29334500	-0.09384700	0.64826900
H	-4.71418700	0.25637400	1.58983700
H	-4.93224500	-0.89053300	0.27129400
C	-2.86750900	-0.62939500	0.88572600
H	-2.93490900	-1.41379400	1.65027000
N	-1.89067100	0.37619100	1.34240000
H	-2.13462900	1.26977100	0.91012700
H	-1.97259300	0.50911900	2.34635500
C	-2.28157500	-1.33387800	-0.33949000
O	-1.11668600	-1.22517900	-0.67935100
O	-3.15187400	-2.10927900	-0.96732500
H	-2.71539300	-2.55635800	-1.71173000
H	4.53687600	-0.40401800	-1.57391500
S	4.56212800	-1.20992300	-0.49265100
C	4.28109000	0.10641600	0.75955600
H	4.60945900	-0.32073700	1.70837500
H	4.91361000	0.96432900	0.53847800
C	2.81001500	0.53849200	0.88406100
H	2.73369200	1.23605400	1.72877500
N	1.85972000	-0.56644200	1.13123700
H	2.15867500	-1.36021400	0.55728700
H	1.95022900	-0.87344900	2.09669100
C	2.38493400	1.36470700	-0.32943500
O	3.10629100	2.02134700	-1.01665500
O	1.02133900	1.32174600	-0.53756300
H	0.82229300	1.89058700	-1.29926300
Li	-0.02576900	-0.07178000	0.43842300



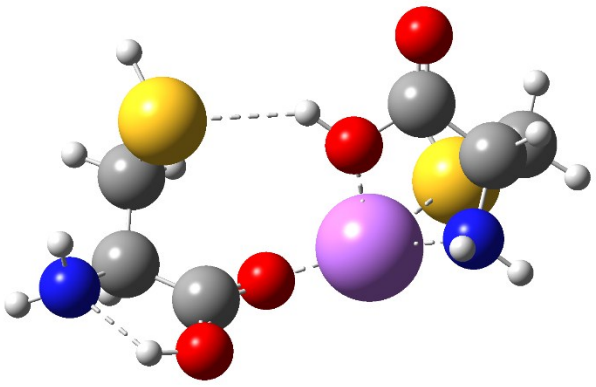
Iso 12 (22.26 kJ/mol)

H	2.83992500	-1.20232500	1.71194800
S	2.07956900	-1.79153200	0.76186100
C	3.09036300	-1.18364400	-0.66124800
H	3.90493500	-1.89197000	-0.81835800
H	2.44552500	-1.22658400	-1.53958500
C	3.68852500	0.21649800	-0.49578800
H	4.25905700	0.42030300	-1.41704300
N	4.51353700	0.28872800	0.71472900
H	5.30463900	-0.34441700	0.64021200
H	4.88871400	1.22192200	0.85135500
C	2.64536300	1.32931700	-0.42187600
O	1.43691300	1.18975100	-0.37138000
O	3.22111000	2.52729500	-0.42686800
H	2.54105800	3.21896400	-0.37337100
H	-4.12233200	2.39462800	0.92262400
S	-4.14992100	1.56848600	-0.14183100
C	-4.02364700	-0.01847500	0.79131700
H	-4.32846700	0.15088500	1.82335100
H	-4.73502700	-0.70965800	0.34249300
C	-2.60866400	-0.62691900	0.76169200
H	-2.63468900	-1.54883300	1.35709800
N	-1.54148000	0.23328800	1.30235900
H	-1.74872300	1.19962700	1.04255900
H	-1.54466800	0.19629700	2.31766500
C	-2.17813800	-1.08332700	-0.63362900
O	-1.03817700	-0.97592500	-1.04844700
O	-3.15285100	-1.65244500	-1.32760300
H	-2.80925600	-1.95281600	-2.18532000
Li	0.21392400	-0.17383500	0.21194800



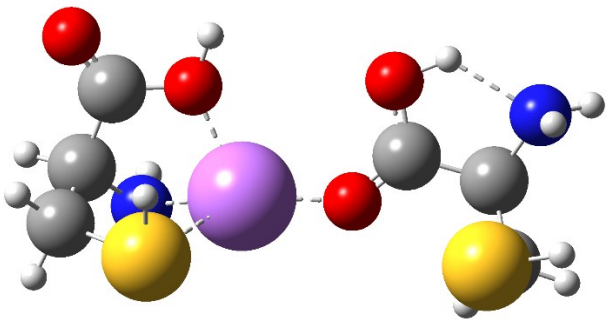
Iso 13 (22.92 kJ/mol)

H	2.38103000	3.00762600	0.87889900
S	2.18356100	1.93684200	0.08631700
C	2.71891000	0.64314900	1.30485800
H	3.51626300	1.06333000	1.91610700
H	1.88030900	0.37552000	1.94507400
C	3.24382700	-0.60853700	0.58431100
H	3.50176400	-1.33437200	1.36420100
N	4.40731200	-0.42494700	-0.28376000
H	4.46855200	0.52234400	-0.64814900
H	5.28169600	-0.65735400	0.17157400
C	2.13642000	-1.30130900	-0.23761800
O	0.98922400	-1.41208400	0.16743800
O	2.52385700	-1.77129800	-1.39571000
H	3.48160500	-1.50930900	-1.47189000
H	-2.47184500	0.02003100	2.27420500
S	-2.81406700	-1.09734500	1.60035700
C	-3.87887500	-0.28298600	0.32525700
H	-4.63760000	-1.02344300	0.06554400
H	-4.38874600	0.56766100	0.77410800
C	-3.13163800	0.14576700	-0.95231800
H	-3.87484800	0.57107100	-1.63567500
N	-2.41446800	-1.01372200	-1.52574100
H	-3.06614500	-1.78234400	-1.66893300
H	-2.05150100	-0.78239200	-2.44836400
C	-2.15775900	1.28169900	-0.63026300
O	-2.46424500	2.42785100	-0.49197900
O	-0.88891800	0.80606000	-0.46669800
H	-0.24823900	1.51567100	-0.24849200
Li	-0.83292600	-1.19540800	-0.15275100



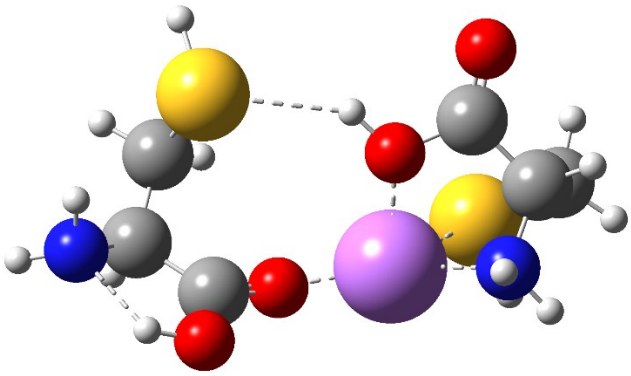
Iso 14 (23.59 kJ/mol)

H	4.94637100	1.53920000	-1.06656900
S	3.66262900	1.68103000	-0.68084300
C	3.76105500	0.67167500	0.85827700
H	4.77609800	0.71277400	1.25097700
H	3.10160400	1.15178000	1.58024000
C	3.32760100	-0.79055300	0.66758600
H	3.43000600	-1.29452700	1.63679200
N	4.05739700	-1.57027100	-0.33463600
H	4.41123500	-0.97857800	-1.08231800
H	4.82488500	-2.10251300	0.05746500
C	1.83016300	-0.89424400	0.33275400
O	0.97118800	-0.22176800	0.88634700
O	1.53152200	-1.79416000	-0.57707900
H	2.41644900	-2.16315200	-0.85879400
H	-2.14620600	1.63685500	-1.68601800
S	-2.14235000	2.03286400	-0.39634800
C	-3.75547700	1.26993400	0.08859300
H	-4.15974800	1.91547000	0.87044000
H	-4.44067400	1.30846700	-0.75647700
C	-3.64627200	-0.16912400	0.63081500
H	-4.65548100	-0.48653900	0.91527900
N	-2.68660200	-0.21365300	1.75399000
H	-2.94811900	0.47639500	2.45497200
H	-2.73381600	-1.11645800	2.22217200
C	-3.21296400	-1.11317700	-0.48953800
O	-3.93010700	-1.55495200	-1.33424600
O	-1.86238500	-1.35902600	-0.44401600
H	-1.61460600	-1.94474900	-1.17830700
Li	-0.87813500	0.00097500	0.72025300



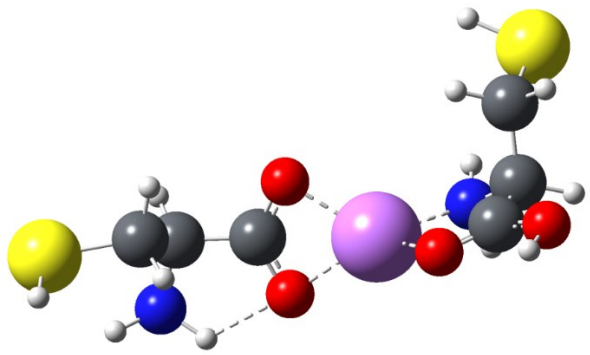
Iso 15 (25.52 kJ/mol)

H	2.30192500	2.95418200	1.05186200
S	2.15430700	1.93567200	0.18305400
C	2.64082900	0.56969200	1.34191000
H	3.40282800	0.95529600	2.01760900
H	1.77417500	0.25700900	1.92162300
C	3.21350800	-0.63004300	0.57110600
H	3.44416300	-1.39955700	1.31701000
N	4.41408600	-0.38352300	-0.22795900
H	4.47829000	0.58348500	-0.53569000
H	5.26919000	-0.62980700	0.25580400
C	2.15513100	-1.28518500	-0.34210000
O	0.99149900	-1.43099400	-0.00059200
O	2.60448400	-1.68676200	-1.50330900
H	3.56099300	-1.41053600	-1.51830400
H	-3.20537100	-2.39252600	1.33744700
S	-2.72129400	-1.15812400	1.57962300
C	-3.83425700	-0.23258300	0.41882200
H	-4.68880700	-0.86975100	0.19202500
H	-4.20623700	0.63865800	0.95676300
C	-3.15419600	0.22083800	-0.89029000
H	-3.93144100	0.67892100	-1.51083900
N	-2.48066100	-0.91796700	-1.54940800
H	-3.14121800	-1.68222600	-1.67353300
H	-2.18475900	-0.65360300	-2.48721100
C	-2.15184500	1.34004800	-0.59113200
O	-2.42607100	2.49734100	-0.48622400
O	-0.89822000	0.83252600	-0.40712700
H	-0.23815200	1.52537000	-0.18850300
Li	-0.82877400	-1.15958100	-0.25640500



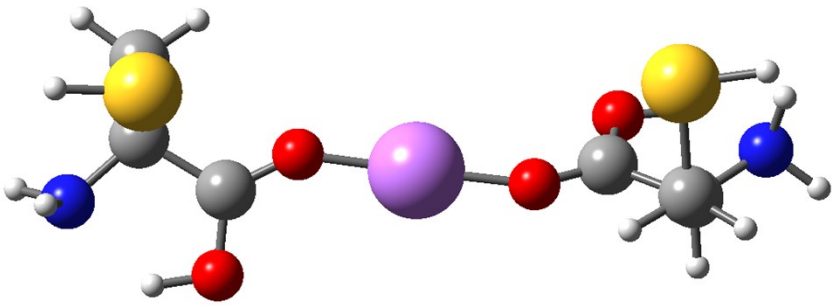
Iso_16 (ZW) (25.54 kJ/mol)

Li	-0.51188000	-0.44814300	0.62514800
H	5.91526000	-1.13655600	-1.29296500
S	5.59130700	0.12840300	-0.96180700
C	3.75900600	-0.12252200	-0.90969500
H	3.30225000	0.23627700	-1.82983200
H	3.55119300	-1.18906800	-0.81344100
C	3.13599300	0.65146100	0.25821000
H	3.23765100	1.72645000	0.10999100
N	3.81227200	0.27666700	1.55901700
H	3.90912500	1.07288800	2.19000800
H	3.14921000	-0.40272600	1.99615400
H	4.75050400	-0.10848000	1.37368400
C	1.64512800	0.26509000	0.43039500
O	0.83592000	0.62791900	-0.43637200
O	1.37744300	-0.44320100	1.44603000
H	-3.36107300	2.87845900	-0.82741000
S	-4.38336400	2.12854300	-0.37201300
C	-3.67905400	0.48976000	-0.84086400
H	-4.40586200	-0.01866000	-1.47235700
H	-2.77206600	0.65532100	-1.42311200
C	-3.37733000	-0.39414700	0.39363700
H	-4.32362100	-0.61674100	0.89763700
N	-2.39201600	0.24361500	1.28264300
H	-2.51662600	-0.09553600	2.23422600
H	-2.60354700	1.24094800	1.31961200
C	-2.78169000	-1.70554300	-0.10371000
O	-1.58724600	-1.94469900	-0.09107500
O	-3.69177700	-2.54207600	-0.58498500
H	-3.25267800	-3.33939900	-0.92476700



Iso_17 (25.56 kJ/mol)

H	5.41633200	-2.34974500	0.12403500
S	4.09569800	-2.08845200	0.05692700
C	4.18638500	-0.71005800	-1.16318800
H	5.06032000	-0.84823400	-1.79829800
H	3.29999800	-0.79795200	-1.79032100
C	4.21976700	0.68534200	-0.51977900
H	4.27511000	1.42174500	-1.33154600
N	5.31037100	0.95448200	0.41846200
H	5.61536600	0.10717300	0.89089000
H	6.10989700	1.39853700	-0.01676500
C	2.90244500	1.01010900	0.20384800
O	1.79985700	0.73164900	-0.25858800
O	3.03539000	1.64503900	1.33673500
H	4.02298700	1.71584100	1.47016800
H	-5.41638200	-2.34958100	-0.12476200
S	-4.09579000	-2.08834600	-0.05664000
C	-4.18739800	-0.70959200	1.16300200
H	-5.06186700	-0.84753300	1.79742800
H	-3.30153600	-0.79734500	1.79089400
C	-4.22017900	0.68561900	0.51915200
H	-4.27616700	1.42226200	1.33065600
N	-5.30998800	0.95452300	-0.42007900
H	-5.61464900	0.10708100	-0.89248300
H	-6.10984500	1.39877200	0.01434300
C	-2.90223000	1.01011000	-0.20346000
O	-1.80004700	0.73174900	0.26000300
O	-3.03418500	1.64467400	-1.33666700
H	-4.02166900	1.71546500	-1.47095600
Li	0.00001100	0.77173100	0.00137800

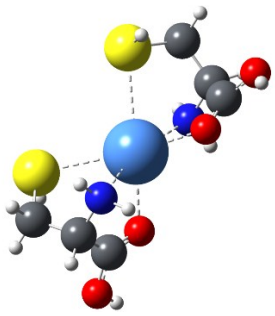


Atomic Coordinates $[(Cys)_2Na]^+$

Note: Energies include thermal correction at 298 K

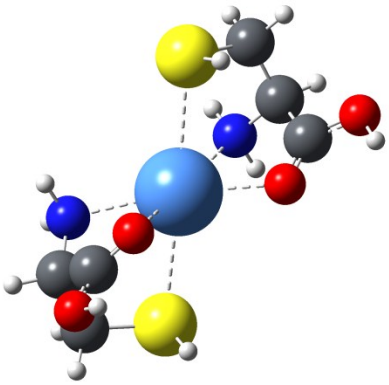
Iso_1 (GM)

H	-2.77435200	-1.67251600	1.61105300
S	-2.29320700	-1.99655700	0.39360700
C	-3.49653700	-1.00869900	-0.59714800
H	-3.63145100	-1.56195300	-1.52837400
H	-4.45600800	-1.00016200	-0.08320200
C	-3.05671600	0.43122900	-0.93901600
H	-3.89308700	0.89186900	-1.48030800
N	-1.80445700	0.42090000	-1.70527700
H	-1.90790000	-0.17520000	-2.52214100
H	-1.59655500	1.35238300	-2.05794700
C	-2.84774800	1.23635000	0.33869100
O	-1.76629500	1.47453000	0.83198700
O	-4.00718900	1.61905300	0.87657300
H	-3.83375800	2.10424600	1.69969700
H	2.77439300	-1.67252800	-1.61101800
S	2.29319100	-1.99656900	-0.39359400
C	3.49648400	-1.00872700	0.59722300
H	3.63133300	-1.56197200	1.52846400
H	4.45598500	-1.00021700	0.08333200
C	3.05667500	0.43121600	0.93904600
H	3.89303300	0.89184600	1.48036700
N	1.80438900	0.42093000	1.70526000
H	1.90778700	-0.17516400	2.52213400
H	1.59650100	1.35242300	2.05791500
C	2.84779100	1.23632100	-0.33868700
O	1.76637600	1.47453700	-0.83204800
O	4.00727200	1.61900500	-0.87649600
H	3.83390100	2.10420600	-1.69962800
Na	-0.00000800	0.06516400	-0.00011100



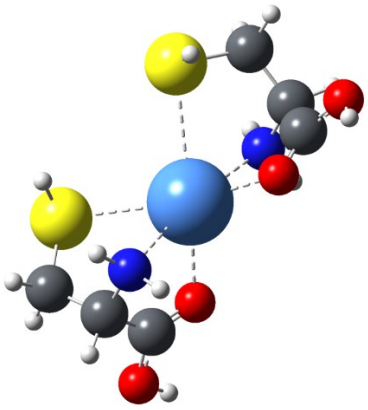
Iso_2 (0.13 kJ/mol)

H	-2.54055000	-2.13953400	1.00565300
S	-2.28280000	-2.05635200	-0.31548500
C	-3.56551700	-0.79669600	-0.72836400
H	-3.84213700	-0.99518400	-1.76553400
H	-4.44868900	-0.97634600	-0.11787500
C	-3.12201300	0.67726300	-0.60915400
H	-4.00238500	1.28591000	-0.85253500
N	-1.97119600	0.94806100	-1.48092600
H	-2.18599900	0.65508000	-2.43040600
H	-1.79453700	1.94894800	-1.52733900
C	-2.73485100	0.99993500	0.83002300
O	-1.59424900	1.07815500	1.23218300
O	-3.80706800	1.15187300	1.60891100
H	-3.51863500	1.32808200	2.51943200
H	2.54081500	2.13967400	1.00564300
S	2.28295700	2.05641200	-0.31547000
C	3.56556500	0.79664500	-0.72834700
H	3.84220600	0.99513400	-1.76551100
H	4.44874900	0.97621800	-0.11785300
C	3.12195200	-0.67729100	-0.60917300
H	4.00228900	-1.28598100	-0.85256900
N	1.97113200	-0.94800100	-1.48096800
H	2.18598600	-0.65505800	-2.43044900
H	1.79438600	-1.94887400	-1.52736700
C	2.73477900	-1.00000800	0.82999300
O	1.59418100	-1.07817700	1.23217400
O	3.80699300	-1.15188800	1.60889700
H	3.51855800	-1.32805600	2.51942600
Na	-0.00004200	-0.00001700	-0.20012500



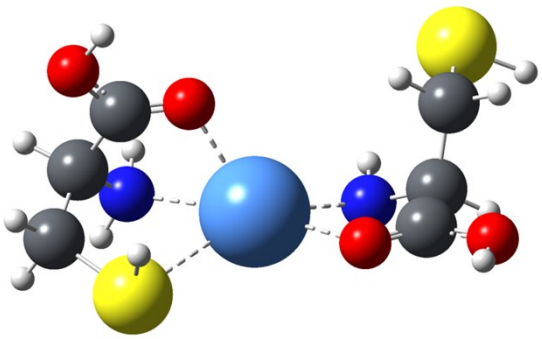
Iso_3 (2.62 kJ/mol)

H	-1.71784600	2.67699800	0.50988600
S	-2.21166100	1.97623500	-0.52976100
C	-3.51036400	1.05546800	0.40722800
H	-3.81881800	1.66659700	1.25566600
H	-4.36860500	0.97024600	-0.25849600
C	-3.10475200	-0.35082900	0.90197700
H	-3.97496600	-0.74785100	1.43992200
N	-1.88796500	-0.30116900	1.72143700
H	-2.00017300	0.38856200	2.45980900
H	-1.74246400	-1.19314300	2.18904800
C	-2.86438200	-1.27159300	-0.29168700
O	-1.77180100	-1.56476900	-0.72793100
O	-4.01090500	-1.69492300	-0.82479900
H	-3.81956000	-2.24551400	-1.60152500
H	2.73133100	1.67493500	1.59866100
S	2.22546300	1.98386200	0.38739600
C	3.44182500	1.02878200	-0.62003900
H	3.53944300	1.57979500	-1.55716700
H	4.41008000	1.05861000	-0.12364300
C	3.04680600	-0.42830000	-0.94282000
H	3.89170000	-0.86440300	-1.49109400
N	1.78488000	-0.46857700	-1.69090600
H	1.84909200	0.13247400	-2.50815000
H	1.60979500	-1.40730900	-2.04208000
C	2.88284700	-1.22677000	0.34613900
O	1.81734600	-1.48486000	0.86353900
O	4.06126700	-1.57666800	0.86441200
H	3.91554900	-2.05863100	1.69487600
Na	-0.01117600	-0.17049900	0.02653100



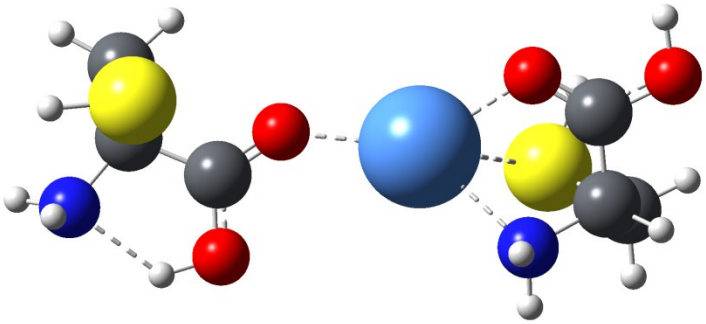
Iso_4 (4.15 kJ/mol)

H	-3.08190200	1.83138100	-1.11543100
S	-3.00112900	1.80779900	0.23070200
C	-3.99880100	0.27926500	0.49935800
H	-4.47472600	0.41140900	1.47283200
H	-4.79180400	0.23598200	-0.24509700
C	-3.20484100	-1.04505200	0.51578100
H	-3.94044900	-1.84564200	0.66451400
N	-2.16486700	-1.01604900	1.55438100
H	-2.58136400	-0.75659200	2.44501700
H	-1.77795800	-1.94774500	1.68668300
C	-2.54430500	-1.28673800	-0.83764800
O	-1.37197000	-1.08477700	-1.07581100
O	-3.42001500	-1.71500200	-1.74590300
H	-2.96946600	-1.83065300	-2.59863500
H	5.17326100	-1.59744200	0.51369000
S	3.98512800	-2.10126600	0.11885500
C	3.32570700	-0.55576500	-0.61777400
H	4.04125200	-0.15441600	-1.33358700
H	2.43618100	-0.87025200	-1.16880200
C	2.95149100	0.52851700	0.42087000
H	3.87493500	0.88205100	0.89267900
N	1.97706300	0.01117800	1.39265400
H	2.27435400	-0.92964700	1.65288000
H	2.02305000	0.56094800	2.24760800
C	2.34064600	1.70746800	-0.33235600
O	1.14851300	1.90713000	-0.45173500
O	3.27285300	2.48123000	-0.88563500
H	2.84344200	3.19142100	-1.39024700
Na	-0.33932700	0.37036000	0.49427400



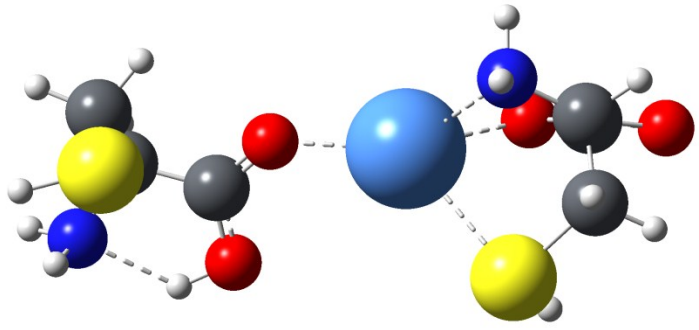
Iso_5 (4.82 kJ/mol)

H	3.54499200	-1.12689300	-1.97895900
S	3.10228900	-1.78788300	-0.88960000
C	4.21032500	-0.97455100	0.34362600
H	4.37657500	-1.72380800	1.11979900
H	5.17232900	-0.77503800	-0.12518400
C	3.65975900	0.30741300	1.00606200
H	4.44765700	0.67295400	1.67608800
N	2.39252600	0.03262200	1.69907300
H	2.50751300	-0.76214300	2.32295000
H	2.13946300	0.81972800	2.29232200
C	3.42132600	1.38485300	-0.04760100
O	2.34017700	1.63355800	-0.53930300
O	4.55109300	1.99563200	-0.39858100
H	4.36207100	2.65093800	-1.09061000
H	-5.53512400	1.86896600	0.49733700
S	-4.20015000	1.88519600	0.31214900
C	-4.13307600	0.65259800	-1.05771500
H	-5.07429300	0.67603000	-1.60534200
H	-3.34354700	0.98695300	-1.72946200
C	-3.82868700	-0.77816500	-0.58773600
H	-3.82615700	-1.42237100	-1.47591200
N	-4.74715600	-1.36044400	0.39276000
H	-5.14288400	-0.64726800	1.00027700
H	-5.50062700	-1.88616200	-0.03361200
C	-2.40028000	-0.89401800	-0.02409900
O	-1.43604600	-0.33806900	-0.52417500
O	-2.28597200	-1.67856000	1.02710000
H	-3.21528200	-1.97161900	1.22751300
Na	0.74593400	-0.06470900	-0.16512400



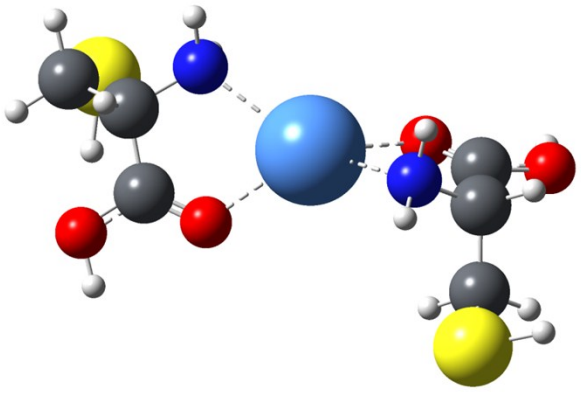
Iso_6 (4.88 kJ/mol)

H	-2.97987500	-0.13653800	-2.36563200
S	-2.45290000	0.96783500	-1.79795800
C	-3.84580100	1.32261900	-0.63906400
H	-3.85112200	2.40739800	-0.51766900
H	-4.78318900	1.04605000	-1.11849200
C	-3.74468500	0.67138000	0.75771100
H	-4.65477900	0.95680100	1.29963700
N	-2.51081000	1.08991500	1.43956200
H	-2.44183800	2.10447100	1.43017700
H	-2.54456900	0.82105600	2.42044200
C	-3.74730000	-0.84912700	0.63317700
O	-2.75067900	-1.54056000	0.66881100
O	-4.97352200	-1.32958800	0.43789600
H	-4.92913600	-2.29454900	0.33350100
H	5.45701600	1.90415100	0.01391600
S	4.13972000	1.82529400	0.28778500
C	4.17577500	0.21141100	1.17936200
H	5.15816700	0.07398300	1.62917200
H	3.44482500	0.29040000	1.98299500
C	3.82633400	-0.99256300	0.29145100
H	3.88755200	-1.89149400	0.91773300
N	4.66216100	-1.20686200	-0.89127300
H	5.00848500	-0.32698300	-1.26580300
H	5.44695300	-1.82253600	-0.71534800
C	2.35826700	-0.94540500	-0.17014900
O	1.43919600	-0.59100700	0.55033800
O	2.15604000	-1.35915900	-1.40383500
H	3.06368300	-1.55591700	-1.75952500
Na	-0.76677700	-0.30864500	0.33627700



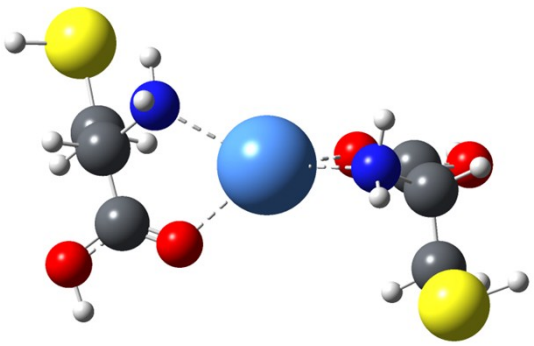
Iso_7 (7.62 kJ/mol)

Na	0.08602000	0.24402000	0.57066600
H	5.67237600	-1.47395000	0.22017600
S	4.50283900	-1.98654800	-0.21672500
C	3.75553200	-0.39883300	-0.75054400
H	4.43587400	0.12271900	-1.42175700
H	2.87211900	-0.68871200	-1.32459700
C	3.34988600	0.53221900	0.41781700
H	4.26505600	0.87301000	0.91409700
N	2.42516400	-0.14726300	1.33841400
H	2.76031200	-1.10406400	1.45792900
H	2.48726200	0.28012200	2.25978800
C	2.66730300	1.76145400	-0.17731100
O	1.46373100	1.91934900	-0.24356000
O	3.54726200	2.63543900	-0.65871200
H	3.07413900	3.37816900	-1.06891800
H	-4.49019100	0.33565100	-1.81311500
S	-4.69136800	1.15826000	-0.76292600
C	-4.58187900	-0.12637600	0.54829700
H	-5.04124400	0.32797500	1.42764300
H	-5.18001200	-0.99151800	0.26926000
C	-3.13666100	-0.53676200	0.90269500
H	-3.19569300	-1.23798800	1.74540800
N	-2.26717800	0.58157500	1.30026400
H	-2.51408100	1.38980400	0.72483600
H	-2.47466500	0.84410000	2.25976200
C	-2.45814900	-1.33722400	-0.21153400
O	-1.29670400	-1.21527800	-0.54461500
O	-3.27638600	-2.23279400	-0.76264500
H	-2.78632400	-2.74771700	-1.42443300



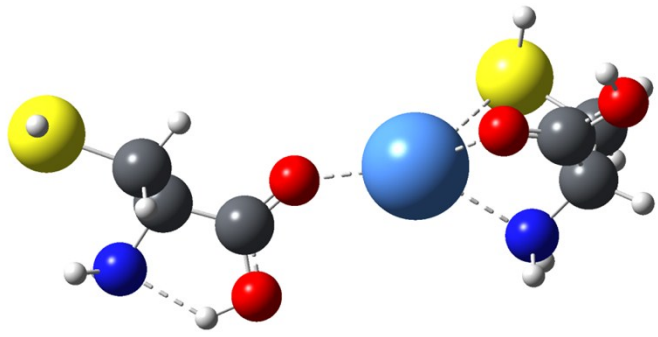
Iso_8 (8.77 kJ/mol)

Na	0.00016500	0.00053000	-0.49701000
H	5.78956500	0.87227700	-0.58642000
S	4.73265500	1.62548000	-0.21610500
C	3.78756000	0.28515800	0.60507600
H	4.41725800	-0.21508200	1.33903800
H	2.98777300	0.80050200	1.14242200
C	3.18821500	-0.75502000	-0.37255400
H	4.01553900	-1.31217800	-0.82520700
N	2.32831500	-0.10482500	-1.37382900
H	2.79582400	0.75442100	-1.66604400
H	2.27966800	-0.68536200	-2.20818900
C	2.36309900	-1.74513800	0.44588100
O	1.15510700	-1.69744400	0.57568200
O	3.12747900	-2.65513600	1.04360600
H	2.57245300	-3.23623300	1.58946700
H	-5.78932000	-0.87305900	-0.58642700
S	-4.73215400	-1.62596800	-0.21624300
C	-3.78744500	-0.28547200	0.60505600
H	-4.41727300	0.21462900	1.33900300
H	-2.98758400	-0.80066600	1.14243700
C	-3.18826400	0.75486700	-0.37253000
H	-4.01573400	1.31172900	-0.82528700
N	-2.32811400	0.10486500	-1.37373200
H	-2.79531500	-0.75458000	-1.66585200
H	-2.27971000	0.68532800	-2.20816000
C	-2.36350100	1.74533500	0.44582200
O	-1.15550300	1.69805700	0.57569000
O	-3.12820600	2.65515600	1.04341100
H	-2.57338600	3.23651400	1.58920400



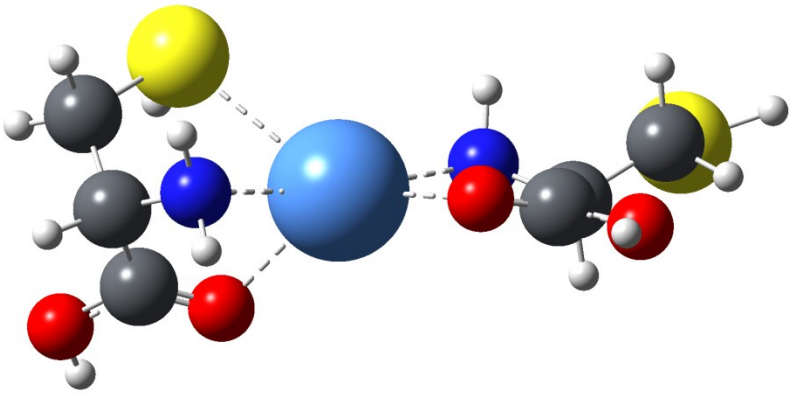
Iso_9 (10.95 kJ/mol)

H	-5.88546200	2.44014500	0.27344500
S	-5.66346800	1.38138200	-0.52960600
C	-4.03063700	0.92218500	0.19616800
H	-3.26120500	1.61203000	-0.14589900
H	-4.09421600	0.96789300	1.28578400
C	-3.65723300	-0.50209100	-0.24565000
H	-3.59983600	-0.52726700	-1.33914300
N	-4.57225900	-1.52176000	0.28496700
H	-5.42243100	-1.10596200	0.65431200
H	-4.85062300	-2.19249100	-0.42317400
C	-2.24253300	-0.81846700	0.27347400
O	-1.24696900	-0.21726200	-0.09731000
O	-2.19139400	-1.78682700	1.16178200
H	-3.13962000	-2.09109500	1.24897700
H	3.33140600	0.98316800	-2.27218900
S	3.05762600	-0.32146600	-2.06605400
C	4.41044800	-0.65664600	-0.85466800
H	4.67733300	-1.70459800	-1.00310100
H	5.28020200	-0.05987100	-1.12374700
C	4.05309500	-0.44516100	0.63294000
H	4.96568700	-0.65584500	1.20406600
N	2.91824500	-1.29546700	1.02144100
H	3.10642400	-2.25944600	0.75790500
H	2.81225000	-1.29829500	2.03354100
C	3.68494600	1.01378000	0.88532400
O	2.54718300	1.43061900	0.95385400
O	4.76303100	1.78886600	0.98049500
H	4.48730800	2.71150900	1.10992600
Na	0.96191100	-0.07842900	0.07353600



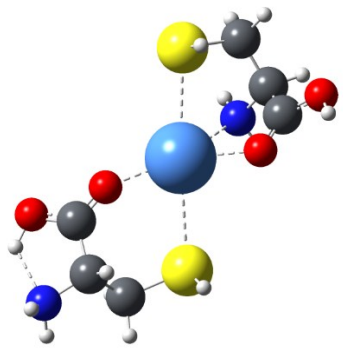
Iso_ 10 (12.79 kJ/mol)

H	5.94137800	-1.76721600	0.04344900
S	4.65798700	-1.80699800	0.45025000
C	4.16951000	-0.18098200	-0.27232300
H	4.92258800	0.56530800	-0.02882000
H	4.09554300	-0.26553300	-1.36001600
C	2.81340300	0.23737400	0.32121800
H	2.94328100	0.36609700	1.40269000
N	1.71996800	-0.72894800	0.11561800
H	1.84660400	-1.20301900	-0.77715500
H	1.77898800	-1.45894200	0.81977000
C	2.37297500	1.61339500	-0.18834900
O	1.23732600	1.89780100	-0.51152200
O	3.37120400	2.49464800	-0.20209100
H	3.03134700	3.35663600	-0.49270900
H	-2.55318400	-2.49738400	-0.34763700
S	-2.40231800	-1.64300800	-1.38029300
C	-3.90206400	-0.61731000	-1.05374100
H	-4.23053500	-0.26570600	-2.03349400
H	-4.68825100	-1.25851300	-0.65920000
C	-3.69304200	0.60622500	-0.13552000
H	-4.67720700	1.07732400	-0.01858200
N	-2.67986900	1.50853700	-0.69722200
H	-2.91446900	1.73313400	-1.66061500
H	-2.67696400	2.39345700	-0.19515300
C	-3.23895500	0.15646300	1.24969300
O	-2.08956000	0.18245000	1.63709500
O	-4.25368600	-0.30901200	1.97696700
H	-3.92138100	-0.60877100	2.83914600
Na	-0.50203300	0.41436400	-0.11901900



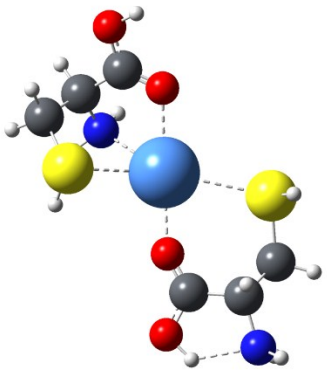
Iso_11 (12.99 kJ/mol)

H	2.99563800	-1.87798000	-1.58203900
S	2.60749100	-2.13767900	-0.31671200
C	3.83659200	-1.05031000	0.52715700
H	4.05070200	-1.53672100	1.48064800
H	4.76071700	-1.04471200	-0.04799600
C	3.37071500	0.39541200	0.80699600
H	4.22027400	0.91191000	1.27104500
N	2.16378300	0.40010400	1.64605200
H	2.31749100	-0.17724100	2.46887100
H	1.98053600	1.33920100	1.99205400
C	3.06519500	1.11334500	-0.50343600
O	1.95048400	1.27684300	-0.95428900
O	4.17711900	1.50893700	-1.12206800
H	3.94372100	1.93073200	-1.96531100
H	-1.87695400	2.62328200	-0.78735400
S	-1.83699300	2.04730400	0.43179800
C	-3.49880100	1.26554000	0.37259300
H	-3.71685400	0.98612500	1.40599900
H	-4.21195000	2.03970000	0.08681600
C	-3.68765600	0.04980300	-0.56434000
H	-3.33138000	0.31403300	-1.56410900
N	-5.10079200	-0.35808000	-0.57451400
H	-5.72064200	0.32539800	-0.15426100
H	-5.44166800	-0.55970400	-1.50803700
C	-2.84315300	-1.15214400	-0.08761200
O	-1.62881100	-1.17207300	-0.15159700
O	-3.53771500	-2.14927200	0.41610500
H	-4.48787100	-1.89266100	0.30120200
Na	0.32757800	-0.15226300	0.04063400



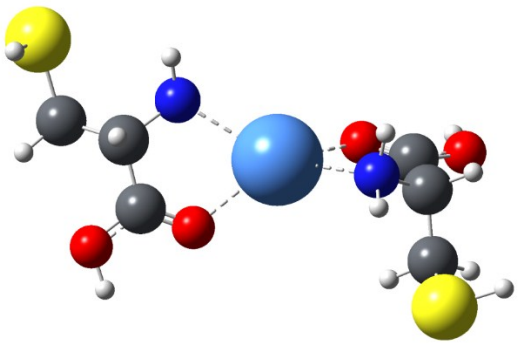
Iso_12 (13.30 kJ/mol)

H	-2.21020800	2.61554700	-1.33573400
S	-1.93400900	2.27794800	-0.05936100
C	-3.47370500	1.32506900	0.27709200
H	-3.50125500	1.21859200	1.36406300
H	-4.31311500	1.95897500	-0.00840900
C	-3.64138500	-0.04897700	-0.40628500
H	-3.39455500	0.04947600	-1.46807600
N	-5.01054700	-0.57363000	-0.30859800
H	-5.50355200	-0.24107100	0.51491400
H	-5.57430800	-0.36080000	-1.12296800
C	-2.67393300	-1.12676700	0.13947000
O	-1.49093100	-0.92757300	0.33995800
O	-3.22699400	-2.30216900	0.34890000
H	-4.18365400	-2.19139400	0.11916000
H	1.47340000	-2.64890800	-0.04619500
S	2.10244300	-1.89972300	-0.97387200
C	3.55898100	-1.41924700	0.05425500
H	3.78379500	-2.23855700	0.73761800
H	4.40015600	-1.33151000	-0.63275000
C	3.41271200	-0.10496900	0.85380500
H	4.35406300	0.02626000	1.40176300
N	2.23263900	-0.13629200	1.72770300
H	2.22240700	-1.00010800	2.26387400
H	2.28262800	0.61700100	2.40971000
C	3.28713500	1.07602100	-0.10634500
O	2.24056700	1.61167500	-0.40672500
O	4.46839200	1.43244700	-0.60810300
H	4.34296100	2.15722200	-1.24247300
Na	0.34768600	0.32411800	0.12539300



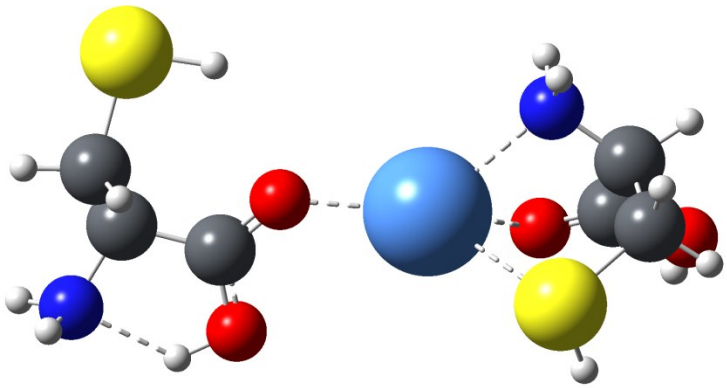
Iso_13 (13.32 kJ/mol)

Na	-0.14613500	-0.35180700	0.13722800
H	-5.67217800	1.33472400	1.09441700
S	-4.58217800	1.94253600	0.58068100
C	-3.97246000	0.51129900	-0.39086100
H	-4.76838500	0.13218500	-1.02975500
H	-3.19280500	0.92628900	-1.03425000
C	-3.39582000	-0.63773100	0.47179800
H	-4.22129300	-1.08774200	1.03391200
N	-2.31474900	-0.15254800	1.34386700
H	-2.60524500	0.75288900	1.71531300
H	-2.23009700	-0.76406200	2.15285400
C	-2.85073400	-1.70519100	-0.47387200
O	-1.67938000	-1.82820600	-0.77585600
O	-3.81826500	-2.47151900	-0.96985900
H	-3.43835300	-3.10538700	-1.60042600
H	5.84508200	-0.09308400	1.63199000
S	5.50244600	-1.00003900	0.69367900
C	4.50859500	0.14003400	-0.34941500
H	5.04149400	1.08032700	-0.47406000
H	4.45545600	-0.33949600	-1.33049200
C	3.08507300	0.38003800	0.19925700
H	3.17838600	0.85325000	1.18435700
N	2.27565600	-0.83756300	0.37228100
H	2.39700900	-1.43421700	-0.44659500
H	2.67534600	-1.37282100	1.14001900
C	2.29513700	1.38909500	-0.63829800
O	1.11244900	1.28824000	-0.90094700
O	3.03466700	2.42649400	-1.02180400
H	2.47789900	3.05250800	-1.51350500



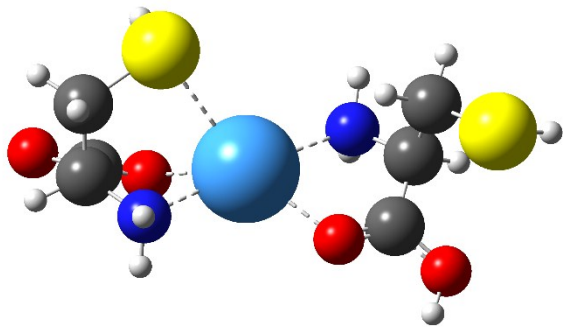
Iso_14 (16.43 kJ/mol)

H	-2.74126800	2.14124500	-0.05321700
S	-4.07901800	2.19302800	-0.19490900
C	-4.42067700	0.53594800	0.51432700
H	-4.06815200	0.49059600	1.54728400
H	-5.51020500	0.47946100	0.53579500
C	-3.90202800	-0.66347800	-0.30145900
H	-4.05477300	-0.44602800	-1.36360700
N	-4.56474400	-1.94365300	0.00506900
H	-4.92442200	-1.97427000	0.95493800
H	-5.33372000	-2.13907100	-0.62547100
C	-2.38608100	-0.88885400	-0.15082700
O	-1.55458900	0.00605700	-0.13935700
O	-2.02880400	-2.15508900	-0.05833700
H	-2.88679100	-2.66183900	-0.05716300
H	3.19955800	-1.70312000	1.59645300
S	2.72394100	-0.50650500	1.99825100
C	4.00590900	0.54204800	1.18127400
H	4.10597800	1.42325200	1.81759400
H	4.95859500	0.01586900	1.20515500
C	3.68406100	1.00599300	-0.25620600
H	4.55123000	1.58518000	-0.59657900
N	2.42903500	1.77226700	-0.28714300
H	2.46653500	2.51691200	0.40449600
H	2.32332400	2.23361400	-1.18808500
C	3.54874500	-0.19856300	-1.18279200
O	2.49002400	-0.68933100	-1.51623400
O	4.73451000	-0.67747900	-1.55185000
H	4.60651800	-1.45913900	-2.11465200
Na	0.69364400	-0.01446800	-0.14923300



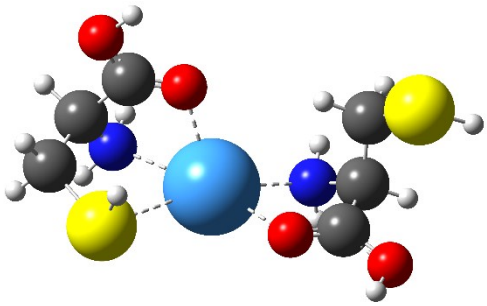
Iso 15 (17.35 kJ/mol)

H	-2.54055000	-2.13953400	1.00565300
S	-2.28280000	-2.05635200	-0.31548500
C	-3.56551700	-0.79669600	-0.72836400
H	-3.84213700	-0.99518400	-1.76553400
H	-4.44868900	-0.97634600	-0.11787500
C	-3.12201300	0.67726300	-0.60915400
H	-4.00238500	1.28591000	-0.85253500
N	-1.97119600	0.94806100	-1.48092600
H	-2.18599900	0.65508000	-2.43040600
H	-1.79453700	1.94894800	-1.52733900
C	-2.73485100	0.99993500	0.83002300
O	-1.59424900	1.07815500	1.23218300
O	-3.80706800	1.15187300	1.60891100
H	-3.51863500	1.32808200	2.51943200
H	2.54081500	2.13967400	1.00564300
S	2.28295700	2.05641200	-0.31547000
C	3.56556500	0.79664500	-0.72834700
H	3.84220600	0.99513400	-1.76551100
H	4.44874900	0.97621800	-0.11785300
C	3.12195200	-0.67729100	-0.60917300
H	4.00228900	-1.28598100	-0.85256900
N	1.97113200	-0.94800100	-1.48096800
H	2.18598600	-0.65505800	-2.43044900
H	1.79438600	-1.94887400	-1.52736700
C	2.73477900	-1.00000800	0.82999300
O	1.59418100	-1.07817700	1.23217400
O	3.80699300	-1.15188800	1.60889700
H	3.51855800	-1.32805600	2.51942600
Na	-0.00004200	-0.00001700	-0.20012500



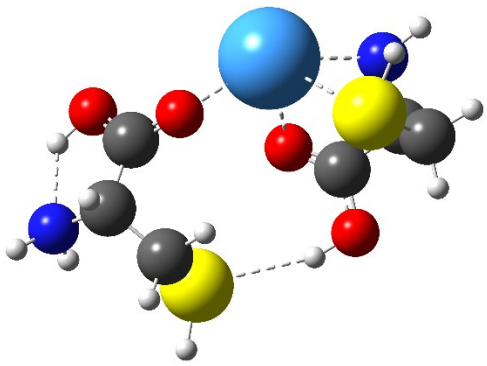
Iso 16 (18.49 kJ/mol)

Na	0.41462400	-0.68541700	0.65195000
H	2.41457600	-0.88248800	-2.19219800
S	2.67994200	-1.64577200	-1.11228800
C	3.92941100	-0.53204100	-0.33755700
H	4.60669500	-1.19136600	0.20857000
H	4.51080100	-0.04782100	-1.12014200
C	3.37004200	0.52055400	0.64419100
H	4.23032700	1.10287000	0.99775400
N	2.62499700	-0.12649300	1.73464100
H	3.20124000	-0.85086900	2.15583500
H	2.43674300	0.54626500	2.47428900
C	2.44185200	1.48804800	-0.08345600
O	1.23000400	1.44421600	-0.03673300
O	3.12212800	2.37279800	-0.81049400
H	2.49990900	2.95119000	-1.28155300
H	-5.04169100	1.32914900	-0.34138400
S	-3.85882900	1.55538900	-0.94979800
C	-2.79185100	1.16875900	0.48640100
H	-1.78350400	1.43682600	0.16274500
H	-3.05495600	1.81863500	1.32365700
C	-2.80551200	-0.29486100	0.97513200
H	-3.80121900	-0.53527800	1.35971600
N	-1.74245800	-0.45722500	1.99464300
H	-1.79335600	0.31562300	2.65433000
H	-1.91627200	-1.29650400	2.54425600
C	-2.50052100	-1.25030700	-0.17790000
O	-1.38111500	-1.44015800	-0.61299700
O	-3.58409800	-1.85504400	-0.64675200
H	-3.34162300	-2.39990000	-1.41398400



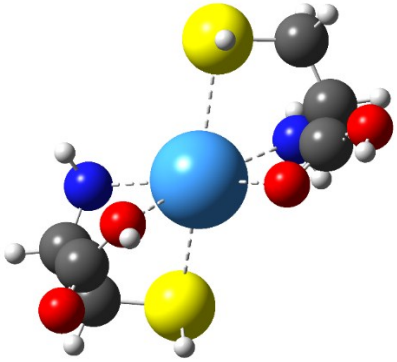
Iso 17 (18.87 kJ/mol)

H	3.56115100	-1.64388200	-1.69886200
S	2.64583200	-0.65754800	-1.77820600
C	3.51628500	0.56343000	-0.69357400
H	4.58482200	0.35205500	-0.73079800
H	3.35859100	1.54113600	-1.14569100
C	3.03351600	0.59293900	0.76895200
H	3.62645100	1.36864100	1.27355600
N	3.15268200	-0.72905400	1.40242100
H	4.10370000	-1.07374600	1.30054400
H	2.98559700	-0.65000800	2.40293100
C	1.57250100	1.03479300	0.85508400
O	0.68827800	0.32518900	1.29054700
O	1.36966000	2.25681600	0.38033300
H	0.40492500	2.43828100	0.37985600
H	-2.69601800	3.08478300	-0.41159700
S	-2.04255900	2.04087000	0.13364300
C	-2.36302600	0.82487600	-1.23357400
H	-1.40876600	0.53051800	-1.66628500
H	-2.94683500	1.33620900	-1.99654900
C	-3.11832800	-0.43004000	-0.75681200
H	-3.36681500	-1.00207800	-1.65850200
N	-4.34568100	-0.20683300	0.00474200
H	-4.32097400	0.67618200	0.50889900
H	-5.18155800	-0.24114400	-0.56582500
C	-2.20479000	-1.38039100	0.04810800
O	-1.06103900	-1.63396600	-0.28570500
O	-2.77135700	-1.92349200	1.10287200
H	-3.68585000	-1.53813100	1.13347600
Na	1.02353800	-1.83552500	0.50038500



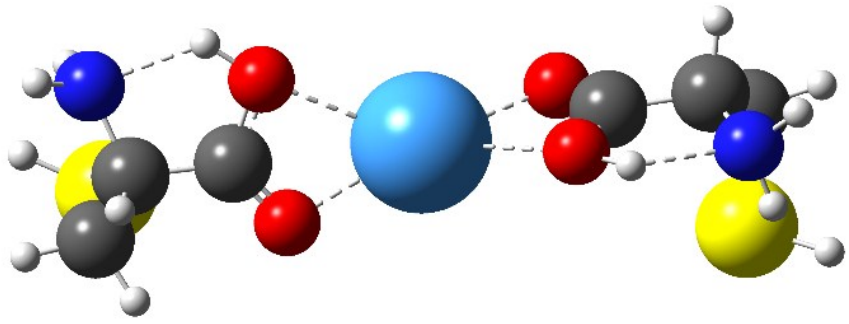
Iso 18 (19.78 kJ/mol)

H	2.67644900	2.23184300	0.76203400
S	2.37614200	1.98580200	-0.52936400
C	3.59561000	0.62653700	-0.79688300
H	3.88635000	0.69852200	-1.84652500
H	4.48389900	0.82701300	-0.20055800
C	3.07690200	-0.80217100	-0.52596900
H	3.92702200	-1.47667000	-0.68879800
N	1.92346300	-1.10694500	-1.38335000
H	2.16236100	-0.92240100	-2.35428400
H	1.70081200	-2.09860900	-1.33347400
C	2.65995700	-0.94451700	0.93404800
O	1.51384400	-0.89676400	1.32889300
O	3.71381400	-1.08909200	1.73679500
H	3.41232400	-1.15100000	2.65802100
H	-2.66880100	-2.26751800	0.50922500
S	-2.30690300	-1.88601000	-0.73279500
C	-3.56218100	-0.54723800	-0.93626900
H	-3.76324900	-0.49290300	-2.00773700
H	-4.48185700	-0.85531700	-0.44265600
C	-3.13256400	0.84125000	-0.42865900
H	-4.00306800	1.49854900	-0.55486600
N	-1.94683000	1.32421400	-1.15603100
H	-2.14158500	1.31812300	-2.15449900
H	-1.76188700	2.29542300	-0.91576900
C	-2.90242200	0.77890100	1.07957600
O	-3.77096200	0.58022100	1.87849000
O	-1.59233800	0.94110200	1.43420000
H	-1.54694700	0.89061400	2.40342300
Na	-0.01388800	0.03513300	-0.25867300



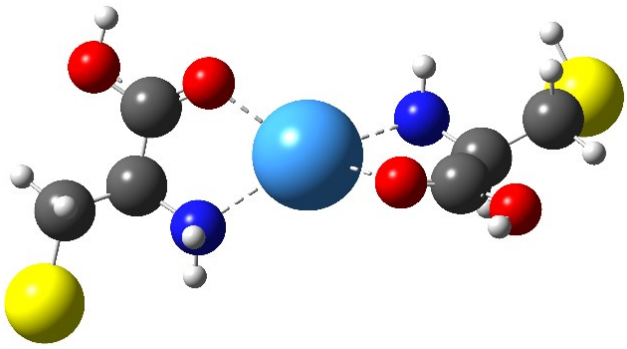
Iso 19 (20.72 kJ/mol)

H	5.95852700	-1.71204800	0.96834800
S	4.73638900	-1.90158500	0.43169000
C	4.87371000	-0.65544300	-0.91882900
H	5.91629600	-0.56204900	-1.21976000
H	4.31344800	-1.05867800	-1.76181900
C	4.30501800	0.72348700	-0.54643200
H	4.44922800	1.38597100	-1.40898800
N	4.87195900	1.37900900	0.63593000
H	5.20289500	0.69640900	1.31368700
H	5.63009700	2.01202500	0.41024000
C	2.78467100	0.65995500	-0.35502600
O	2.01296700	0.03531200	-1.05588600
O	2.32251300	1.39266900	0.66007800
H	3.13666100	1.77666400	1.09103300
H	-5.95823000	-1.71237000	-0.96835200
S	-4.73611100	-1.90171900	-0.43157900
C	-4.87366500	-0.65547400	0.91881500
H	-5.91627800	-0.56218900	1.21968800
H	-4.31339700	-1.05857400	1.76186500
C	-4.30511500	0.72351700	0.54639900
H	-4.44948900	1.38598400	1.40892900
N	-4.87206600	1.37883200	-0.63608700
H	-5.20355500	0.69619500	-1.31351900
H	-5.62972600	2.01243800	-0.41046300
C	-2.78474100	0.66010300	0.35505100
O	-2.01298800	0.03592000	1.05627900
O	-2.32271000	1.39229700	-0.66045100
H	-3.13698000	1.77598800	-1.09154300
Na	-0.00006400	0.44416000	-0.00000300



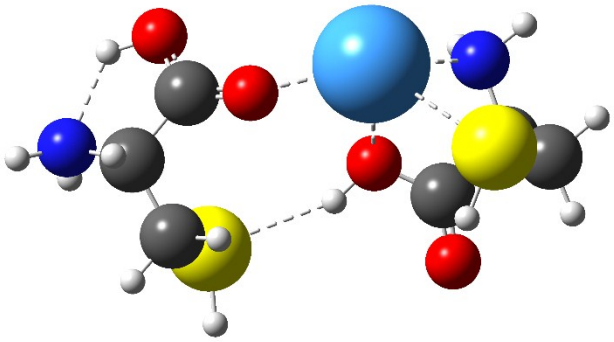
Iso 20 (21.07 kJ/mol)

Na	0.00156500	0.04101100	0.30025800
H	-5.67137200	-0.41083000	-2.11496000
S	-5.36084400	-1.29693300	-1.14606600
C	-4.69697100	-0.07435500	0.05393300
H	-5.36091500	0.78600700	0.10503200
H	-4.73344500	-0.57478300	1.02528900
C	-3.24965400	0.36225000	-0.26156300
H	-3.25121600	0.85226700	-1.24289500
N	-2.27131900	-0.73626200	-0.32143600
H	-2.44161300	-1.37326800	0.45730800
H	-2.47096400	-1.28902700	-1.15220200
C	-2.73570500	1.43532600	0.70192300
O	-1.60232100	1.48000900	1.13981800
O	-3.65582700	2.35376500	0.98410600
H	-3.26779100	3.02822900	1.56563100
H	5.06090700	2.29219700	-0.69680700
S	5.44057900	1.11632500	-1.23613800
C	4.70913000	0.02053300	0.04528400
H	5.33079700	-0.87340000	0.05963400
H	4.79835900	0.49574000	1.02452200
C	3.24525700	-0.36700000	-0.25361100
H	3.23110300	-0.87420900	-1.22574000
N	2.30003800	0.75862100	-0.33756400
H	2.49984600	1.42458600	0.40842000
H	2.48153500	1.26130300	-1.20306200
C	2.70252500	-1.40340400	0.73394300
O	1.56981600	-1.40558700	1.17598100
O	3.59625400	-2.34182300	1.03355500
H	3.18988400	-2.99371500	1.62810900



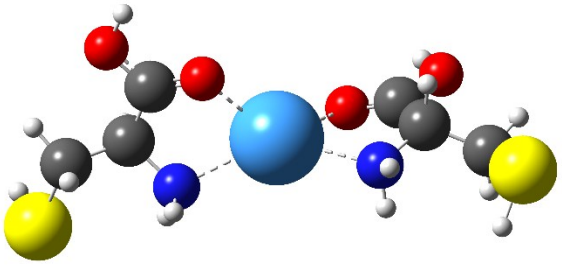
Iso 21 (21.16 kJ/mol)

H	-2.52540200	0.13012800	2.27593700
S	-3.06157900	-0.91057800	1.60586600
C	-3.97483900	0.08121600	0.34022400
H	-4.84485400	-0.52056400	0.07166000
H	-4.33529900	0.99323800	0.81194300
C	-3.17742500	0.42528700	-0.92957600
H	-3.83361500	1.05444300	-1.54496200
N	-2.75495100	-0.80245800	-1.63190100
H	-3.57454300	-1.37167600	-1.83127600
H	-2.35868800	-0.56228800	-2.53789900
C	-1.99151500	1.32246400	-0.56457100
O	-2.11362000	2.43070800	-0.12457700
O	-0.79434800	0.71508400	-0.75947700
H	-0.05525400	1.31829000	-0.51479700
H	2.14461800	3.09888600	0.59239700
S	2.20584800	1.95954300	-0.12372000
C	2.77235600	0.85268400	1.25357600
H	3.50147800	1.39997300	1.84952800
H	1.92270400	0.58491700	1.87889200
C	3.42742900	-0.41960600	0.69564900
H	3.71055700	-1.03019700	1.56056700
N	4.60988000	-0.23005300	-0.14631100
H	4.61680800	0.67809300	-0.60305400
H	5.47879200	-0.34508600	0.36119100
C	2.41256600	-1.29175000	-0.07628300
O	1.26823000	-1.46629900	0.30590700
O	2.88540700	-1.84350600	-1.17037000
H	3.81801900	-1.50798800	-1.24755800
Na	-0.88499300	-1.63506400	-0.24685500



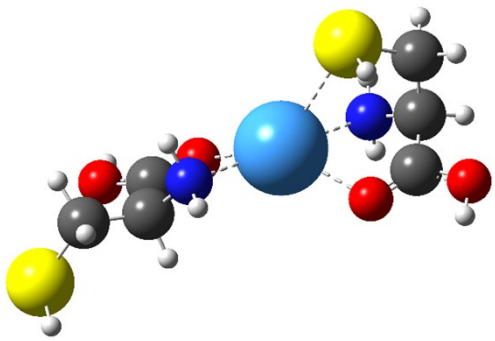
Iso 22 (21.51 kJ/mol)

Na	-0.00183600	0.05802400	0.00766100
H	-5.86067300	-0.35759600	-1.74577600
S	-5.41976300	-1.39837100	-1.00902800
C	-4.67713800	-0.40134100	0.34371100
H	-5.36364300	0.39138800	0.63357400
H	-4.59045100	-1.08582700	1.19180500
C	-3.29011400	0.17360000	-0.01631600
H	-3.41612900	0.85032700	-0.87040500
N	-2.28416600	-0.83182800	-0.39968600
H	-2.33677900	-1.61410800	0.25307300
H	-2.56323200	-1.22579100	-1.29578300
C	-2.71171800	1.05781300	1.09179400
O	-1.53624300	1.08959700	1.40009000
O	-3.63054400	1.83112300	1.66388900
H	-3.20359900	2.39921200	2.32626900
H	4.97004500	-2.49875000	0.76849800
S	5.48909100	-1.28217000	1.02978900
C	4.68043800	-0.37786600	-0.35082200
H	5.35293300	0.44107100	-0.60151400
H	4.61909700	-1.02862500	-1.22573800
C	3.29239800	0.18341000	0.02355500
H	3.42905800	0.85803300	0.87729700
N	2.29281200	-0.82223900	0.42175900
H	2.35602800	-1.62546500	-0.20305400
H	2.54789400	-1.17450300	1.34147300
C	2.70133700	1.06661400	-1.07901400
O	1.52326800	1.09653900	-1.37819700
O	3.61342700	1.84212300	-1.65860900
H	3.17939800	2.41105500	-2.31551700



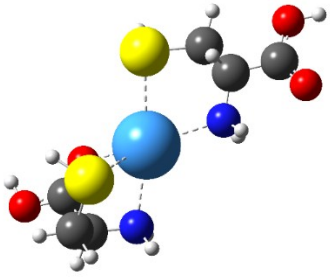
Iso 23 (22.09 kJ/mol)

Na	-0.57535200	0.21237100	0.10409100
H	-3.12159500	-0.21380800	-2.35307600
S	-2.88156200	0.97546500	-1.76389800
C	-4.15116200	0.83336300	-0.43079700
H	-4.46909100	1.85700500	-0.22472700
H	-5.01448800	0.29852800	-0.82260200
C	-3.67269000	0.19103700	0.88927100
H	-4.54838800	0.15237600	1.54946100
N	-2.54927800	0.94691600	1.45608300
H	-2.79176900	1.93217600	1.51936800
H	-2.36126200	0.64201300	2.40831800
C	-3.22552900	-1.24707100	0.64550100
O	-2.06935900	-1.59574800	0.52717400
O	-4.26243600	-2.07677000	0.53690800
H	-3.93941600	-2.97507900	0.35747200
H	5.50557400	-2.07689500	-0.15121800
S	5.44527400	-0.75671900	0.11546000
C	4.01819800	-0.39412500	-0.99366000
H	4.22737200	0.56083000	-1.47844000
H	3.99034900	-1.15782900	-1.77046900
C	2.65076000	-0.35882900	-0.28335900
H	2.60995300	-1.19856800	0.41976200
N	1.48474000	-0.49399900	-1.18456600
H	1.59588900	0.12126400	-1.98921000
H	1.45991900	-1.43865700	-1.55906600
C	2.41710800	0.88237600	0.58798900
O	1.31634200	1.22374900	0.97714000
O	3.52659600	1.54441800	0.89044600
H	3.30894700	2.28450800	1.48081200



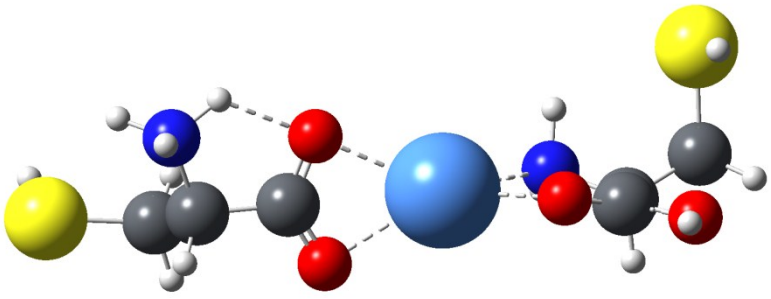
Iso 24 (22.29 kJ/mol)

H	-2.86624600	1.71298800	1.40599700
S	-2.44859600	0.54080400	1.92632400
C	-3.75361600	-0.52869000	1.17828000
H	-3.89690000	-1.34742400	1.88589800
H	-4.68721900	0.02951400	1.13640900
C	-3.42288000	-1.12619200	-0.20644200
H	-4.30236400	-1.70780900	-0.51011100
N	-2.19192500	-1.92832700	-0.14871700
H	-2.26066700	-2.60221400	0.60978500
H	-2.09416900	-2.47600800	-1.00066400
C	-3.23881200	-0.01564800	-1.23604300
O	-2.16225600	0.38872400	-1.62323600
O	-4.40526800	0.48697100	-1.63617100
H	-4.24722500	1.20686100	-2.26908600
H	1.67856600	2.50938700	-1.21981000
S	1.37152500	2.14528300	0.04278400
C	2.89386500	1.17021200	0.38570800
H	3.75818200	1.80147900	0.18644500
H	2.86497900	0.97969200	1.46144600
C	3.01415100	-0.15673400	-0.38771300
H	2.98873300	0.05715900	-1.45927400
N	1.92042100	-1.08613700	-0.06346500
H	1.97598900	-1.87896500	-0.70041700
H	2.12209500	-1.49447100	0.85054900
C	4.38331100	-0.77689900	-0.06604200
O	4.53366900	-1.72751700	0.65584000
O	5.37951400	-0.11091100	-0.67123300
H	6.22592600	-0.51655600	-0.42185400
Na	-0.37703700	-0.16765300	-0.16216800



Iso_25 (ZW) (22.35 kJ/mol)

Na	-0.35642500	-0.38887000	0.05941300
H	6.41962400	1.97905600	0.47926500
S	6.30072700	0.63893400	0.41223800
C	4.47378800	0.56691700	0.69843200
H	4.26236500	0.35415700	1.74436300
H	4.03925600	1.53538200	0.44624300
C	3.83556900	-0.54073000	-0.14456400
H	4.18637600	-1.52233100	0.17328500
N	4.17404700	-0.35443400	-1.60800500
H	4.35499400	-1.24014600	-2.08084800
H	3.28828900	0.05169000	-1.99848200
H	5.00338400	0.24583500	-1.71583800
C	2.28361400	-0.46811900	-0.06143200
O	1.75317700	-0.77134900	1.01499100
O	1.71140000	-0.06964500	-1.11941300
H	-5.24621800	0.40923100	-1.61272700
S	-4.98160800	1.55395200	-0.94977800
C	-4.85381700	0.81269700	0.72856900
H	-4.95107800	1.65452700	1.41600400
H	-5.69375900	0.14253700	0.90035100
C	-3.50918600	0.10582700	1.00062400
H	-3.52064600	-0.22026900	2.04897500
N	-2.32374000	0.95130800	0.80043500
H	-2.49900500	1.55656700	-0.00380800
H	-2.20495700	1.56489600	1.60141100
C	-3.34738700	-1.19009000	0.20212700
O	-2.31111200	-1.56705100	-0.30383300
O	-4.47466600	-1.90209500	0.15472500
H	-4.30188000	-2.73574400	-0.31241300

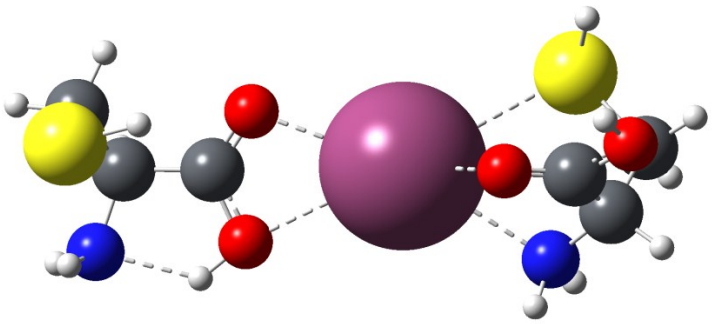


Atomic Coordinates $[(Cys)_2K]^+$

Note: Energies include thermal correction at 298 K

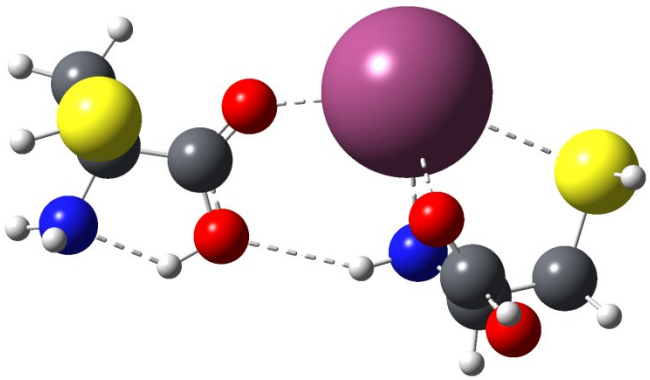
Iso_1 (GM)

H	-3.72465900	2.08637600	-0.59950700
S	-4.99684700	1.72264400	-0.33759600
C	-4.87533800	0.01456100	-1.00858800
H	-5.90716200	-0.30619200	-1.15728600
H	-4.38367900	0.03633300	-1.97983500
C	-4.16794200	-0.98006800	-0.07394900
H	-4.25613200	-1.97601200	-0.52554900
N	-4.67452400	-1.04950800	1.30078000
H	-5.07796700	-0.15729500	1.58154000
H	-5.36953100	-1.77604100	1.42554800
C	-2.65444000	-0.72117000	-0.00635400
O	-1.95684800	-0.43182000	-0.95528300
O	-2.13149300	-0.87788300	1.21293800
H	-2.91826800	-1.07334000	1.79548100
H	3.74998200	-0.25797300	-2.35409600
S	3.47780600	-1.28117900	-1.51908900
C	4.66420400	-0.81086900	-0.18565800
H	5.00686900	-1.75291500	0.24614800
H	5.52714700	-0.33069000	-0.64272300
C	4.09803100	0.07310000	0.94373500
H	4.95192500	0.32616800	1.58772000
N	3.02174000	-0.61704900	1.66448800
H	3.36014700	-1.51798400	1.99231900
H	2.77164600	-0.09084400	2.49842600
C	3.56994500	1.39140500	0.38780100
O	2.40030500	1.69981600	0.32046900
O	4.56493700	2.17193200	-0.04204800
H	4.19387700	2.99727400	-0.39414200
K	0.58568300	-0.31066000	0.04450000



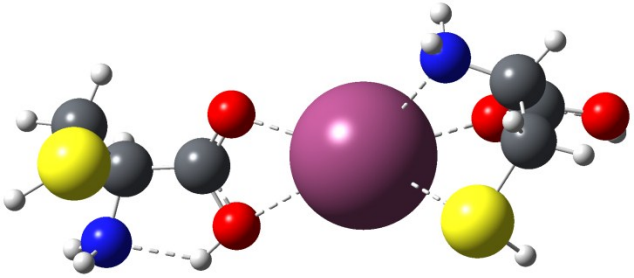
Iso_2 (0.57 kJ/mol)

H	-5.40210900	-1.24710400	1.41035600
S	-4.21885200	-0.63469800	1.61277200
C	-4.43116700	0.71135500	0.36880500
H	-5.49465700	0.87820600	0.20373100
H	-4.01281300	1.61291800	0.81416700
C	-3.72483500	0.42975500	-0.96591700
H	-3.93565500	1.27379200	-1.63436800
N	-4.09851700	-0.80457100	-1.66149600
H	-4.36200200	-1.53284300	-1.00167200
H	-4.85353500	-0.67152200	-2.32369000
C	-2.19206100	0.44052600	-0.80480000
O	-1.59128300	1.23318200	-0.10818900
O	-1.56722100	-0.47675200	-1.53438200
H	-2.30266600	-0.98962500	-1.96841500
H	4.76051100	0.63601800	1.22679000
S	4.26685000	1.25089600	0.13302500
C	4.12492000	-0.25108400	-0.93080200
H	4.31037300	0.09578900	-1.94888300
H	4.92659100	-0.93954200	-0.67044700
C	2.76130100	-0.97329600	-0.89867000
H	2.87940400	-1.87458200	-1.51669800
N	1.69382100	-0.08601700	-1.36326000
H	1.91206200	0.24742200	-2.29802200
H	0.80532700	-0.57879300	-1.43444400
C	2.44808600	-1.45355500	0.51348500
O	1.62719400	-0.95742900	1.25370400
O	3.21887300	-2.48947800	0.85936000
H	3.00374500	-2.75484600	1.76815700
K	0.86380900	1.59585700	0.79775900



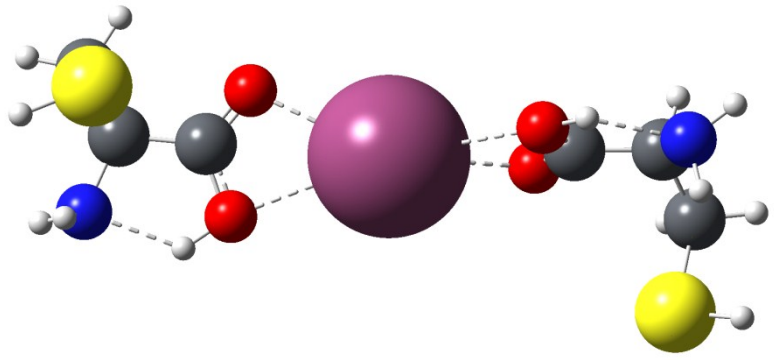
Iso_3 (1.20 kJ/mol)

H	-5.84042300	1.88909300	0.18218200
S	-4.62296800	1.80007100	-0.38964300
C	-4.78306600	0.07663200	-1.02529700
H	-5.83280200	-0.13525300	-1.22401600
H	-4.24669900	0.05192900	-1.97310100
C	-4.19429500	-0.98522400	-0.08357700
H	-4.36094800	-1.96567300	-0.54665100
N	-4.72810500	-1.02989000	1.28067500
H	-5.02567200	-0.10787300	1.59051800
H	-5.50276700	-1.67514400	1.37962300
C	-2.66468800	-0.85571000	0.00867400
O	-1.93510800	-0.61189000	-0.92831700
O	-2.16895600	-1.07219200	1.22997400
H	-2.96684600	-1.21903300	1.80568800
H	3.72668700	0.63340200	2.30646800
S	3.03914400	1.48833500	1.52244800
C	4.20594400	1.47483500	0.09223400
H	4.14615800	2.47433700	-0.34218000
H	5.21770900	1.34568100	0.47149100
C	3.91340200	0.43859700	-1.01165900
H	4.74811800	0.50977700	-1.72303700
N	2.60728500	0.68509700	-1.63211100
H	2.56438000	1.64592300	-1.96144100
H	2.49753500	0.09987400	-2.45692200
C	3.94548800	-0.97739600	-0.44607200
O	2.97615700	-1.68639600	-0.28751300
O	5.18838900	-1.34334900	-0.11982300
H	5.17055000	-2.24422000	0.24192200
K	0.57217900	-0.46439800	0.11706600



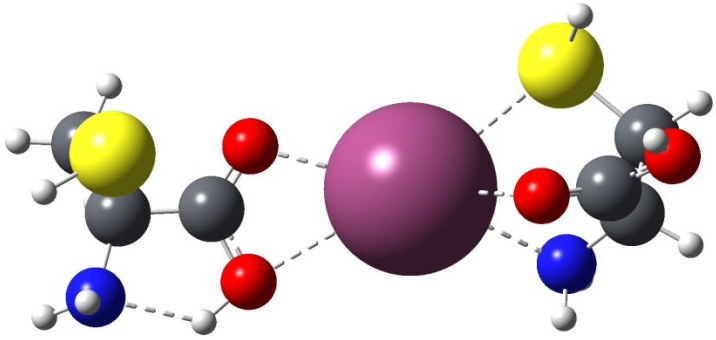
Iso_4 (2.06 kJ/mol)

H	-6.49414200	-0.93728700	-1.56266800
S	-5.34084200	-1.41067500	-1.04975200
C	-5.43849000	-0.55998400	0.58297800
H	-6.48444200	-0.41270300	0.84868100
H	-4.99763500	-1.24359400	1.30760300
C	-4.68461800	0.77837100	0.62711100
H	-4.82273500	1.20248400	1.62935800
N	-5.07667300	1.79265500	-0.35576600
H	-5.41785400	1.36390000	-1.21272400
H	-5.78120900	2.43025900	-0.00455000
C	-3.16797700	0.56197700	0.50342000
O	-2.54888800	-0.32913700	1.04481400
O	-2.54219200	1.47649900	-0.24330700
H	-3.26892700	2.06582900	-0.58419400
H	6.49697700	0.92631600	-1.56454700
S	5.34527200	1.40443600	-1.05243500
C	5.44045200	0.55671300	0.58197500
H	6.48597200	0.40691100	0.84796600
H	5.00160000	1.24305200	1.30523600
C	4.68266900	-0.77934800	0.62880200
H	4.81962200	-1.20187700	1.63187600
N	5.07165300	-1.79672100	-0.35209700
H	5.41406100	-1.37066500	-1.20991200
H	5.77432500	-2.43570600	0.00034100
C	3.16666800	-0.55874100	0.50482100
O	2.55018400	0.33514500	1.04456600
O	2.53812900	-1.47288300	-0.24018100
H	3.26309400	-2.06503500	-0.57993700
K	0.00028800	0.00450000	0.22714400



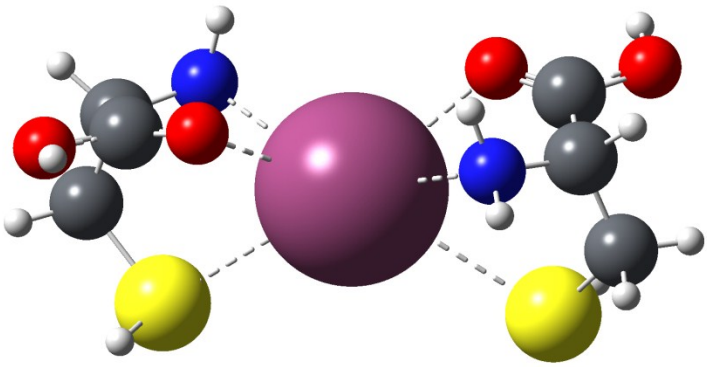
Iso_5 (2.14 kJ/mol)

H	3.57300900	0.30082600	-2.40042100
S	3.35404600	-0.89279100	-1.81252700
C	4.62021400	-0.72712400	-0.48014300
H	4.98841600	-1.73863400	-0.29947500
H	5.45379000	-0.14227200	-0.86389200
C	4.12474900	-0.13621400	0.85513300
H	5.01679300	-0.02591000	1.48759600
N	3.09562300	-0.98992100	1.46036800
H	3.45424300	-1.93698900	1.55031800
H	2.89694800	-0.67361500	2.40658100
C	3.56244700	1.26671800	0.65177800
O	2.39094600	1.56510300	0.72789900
O	4.52869200	2.14025000	0.35489200
H	4.13533200	3.01851700	0.22552500
H	-5.86292800	1.94041000	0.01573200
S	-4.64231100	1.80601800	-0.54029500
C	-4.79935800	0.03668800	-1.03500900
H	-5.84838700	-0.19145300	-1.21887900
H	-4.26010200	-0.06449500	-1.97607600
C	-4.21281600	-0.94486200	-0.00844000
H	-4.38104200	-1.95984800	-0.38921500
N	-4.74743200	-0.87567300	1.35461000
H	-5.52409500	-1.50842200	1.50526500
H	-5.04334800	0.06968000	1.58602700
C	-2.68304600	-0.81103100	0.07348800
O	-1.95361300	-0.64682000	-0.88055200
O	-2.18753000	-0.92672900	1.30858400
H	-2.98604200	-1.02273800	1.89390600
K	0.56111700	-0.35668500	0.10473100



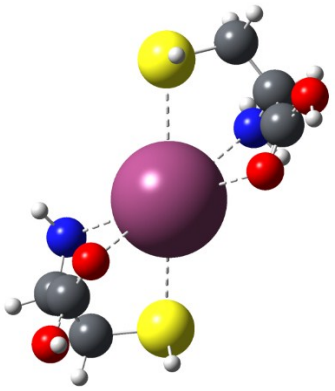
Iso_6 (3.90 kJ/mol)

H	3.39433000	2.08803000	1.05551400
S	2.89354300	2.04045600	-0.19535400
C	4.02122700	0.72994800	-0.84148700
H	4.19116100	0.97903000	-1.89041800
H	4.97747600	0.81142000	-0.32876700
C	3.49053300	-0.71498000	-0.75698600
H	4.31777600	-1.36234400	-1.08212000
N	2.27994200	-0.87712100	-1.56731900
H	2.47344400	-0.59990200	-2.52582600
H	2.01081200	-1.85721000	-1.60361100
C	3.18710900	-1.09903500	0.68692000
O	2.08084500	-1.29318100	1.13958800
O	4.30702500	-1.18376400	1.41310800
H	4.07670400	-1.42704000	2.32414600
H	-3.39134600	2.08772100	-1.05729400
S	-2.89389000	2.04013700	0.19490100
C	-4.02335200	0.72969100	0.83805400
H	-4.19611500	0.97882900	1.88651000
H	-4.97820700	0.81116800	0.32274400
C	-3.49247700	-0.71525100	0.75504900
H	-4.32061600	-1.36258000	1.07796200
N	-2.28410700	-0.87742800	1.56870200
H	-2.48025300	-0.60018900	2.52666800
H	-2.01518500	-1.85754800	1.60575900
C	-3.18513800	-1.09940900	-0.68800600
O	-2.07767100	-1.29378100	-1.13761300
O	-4.30307600	-1.18395700	-1.41726600
H	-4.07030800	-1.42734500	-2.32765000
K	0.00003300	0.12536900	0.00369200



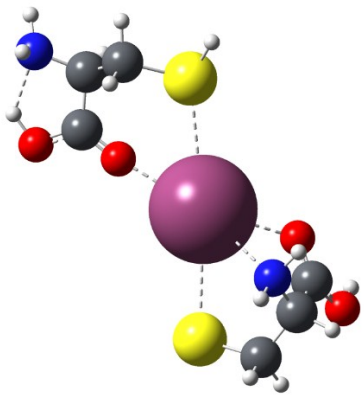
Iso_7 (4.37 kJ/mol)

H	-3.21758200	-2.24539000	0.78674100
S	-2.78824100	-1.99561100	-0.46670500
C	-4.00745800	-0.66905900	-0.86617400
H	-4.20513600	-0.76524200	-1.93524800
H	-4.93707600	-0.88404500	-0.34310300
C	-3.55279500	0.77471600	-0.57505500
H	-4.42652600	1.41300400	-0.77052700
N	-2.38616600	1.13382800	-1.38799000
H	-2.60490900	0.99695100	-2.37116100
H	-2.17878700	2.12356400	-1.27898500
C	-3.21304300	0.95246300	0.90077400
O	-2.10200800	1.14459200	1.34124600
O	-4.30500700	0.85488600	1.66676500
H	-4.05123900	0.97205400	2.59647000
H	3.21777900	2.24538200	0.78670300
S	2.78844700	1.99562100	-0.46675000
C	4.00753100	0.66892900	-0.86615600
H	4.20522400	0.76505500	-1.93523200
H	4.93716500	0.88384100	-0.34308400
C	3.55273900	-0.77480600	-0.57500500
H	4.42642100	-1.41316100	-0.77046600
N	2.38608200	-1.13382900	-1.38793800
H	2.60487000	-0.99709100	-2.37111700
H	2.17854500	-2.12352100	-1.27882900
C	3.21296000	-0.95248000	0.90082400
O	2.10187400	-1.14431500	1.34129800
O	4.30494800	-0.85518200	1.66680900
H	4.05115100	-0.97225000	2.59651900
K	-0.00003400	0.00011900	-0.03400500



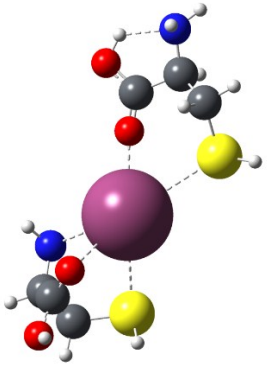
Iso_8 (7.04 kJ/mol)

H	2.97936900	-3.29411700	0.53743100
S	2.55518200	-2.10031100	0.07770100
C	4.02373700	-1.12069400	0.63592200
H	3.86104200	-0.76500100	1.65561000
H	4.87789500	-1.79620000	0.63325000
C	4.34154100	0.05591100	-0.30211500
H	4.36951800	-0.31866500	-1.33120300
N	5.62387300	0.71453200	-0.02959800
H	5.86895900	0.70659900	0.95624600
H	6.39149200	0.30776900	-0.55089600
C	3.23428800	1.12951900	-0.29673300
O	2.05172700	0.85362600	-0.23711000
O	3.66577000	2.37087400	-0.39101100
H	4.65216100	2.31315400	-0.38195500
H	-3.36197600	2.19928000	-1.12735100
S	-2.92368600	2.12859000	0.14584600
C	-4.23529400	0.99318300	0.77472200
H	-4.40400400	1.28618000	1.81254500
H	-5.15602900	1.18854900	0.22866700
C	-3.90125200	-0.51146900	0.73491700
H	-4.81529100	-1.03404200	1.05076200
N	-2.74420000	-0.81701700	1.58405100
H	-2.91718100	-0.47394200	2.52523600
H	-2.63218500	-1.82457400	1.66701700
C	-3.61526300	-0.96678100	-0.69204600
O	-2.52911400	-1.29715500	-1.11366100
O	-4.72143500	-0.94124500	-1.44193300
H	-4.50153400	-1.23073400	-2.34219700
K	-0.33136900	-0.12453400	0.02898100



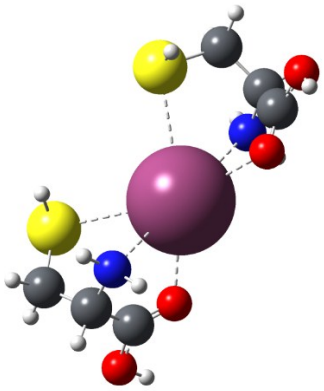
Iso_9 (8.06 kJ/mol)

H	3.05015300	3.22359000	-0.86770500
S	2.61483100	2.10542500	-0.25408700
C	4.01461800	1.01324200	-0.77890000
H	3.79460700	0.57758900	-1.75588500
H	4.89635700	1.64611700	-0.86805100
C	4.32014800	-0.08924500	0.24905400
H	4.39620200	0.37183100	1.23992700
N	5.56820400	-0.81854700	-0.00257200
H	5.78037500	-0.90565000	-0.99225800
H	6.36680600	-0.39742700	0.45721800
C	3.17583900	-1.11615100	0.37188300
O	2.00212300	-0.80346400	0.32308400
O	3.56716300	-2.36005900	0.56387300
H	4.55427400	-2.33973300	0.51938700
H	-3.83736100	2.20498300	0.12511800
S	-3.26587600	1.59077000	1.18072800
C	-4.27513200	0.04673900	1.11867500
H	-4.37810100	-0.27658300	2.15603100
H	-5.27010800	0.29704700	0.75602300
C	-3.68309600	-1.11555100	0.29609900
H	-4.44975100	-1.90326000	0.28833400
N	-2.40561800	-1.56057800	0.86093300
H	-2.53130200	-1.79871400	1.84106400
H	-2.09605600	-2.41301500	0.40032000
C	-3.47591100	-0.69923200	-1.15621700
O	-2.40055800	-0.51497100	-1.68206200
O	-4.64300400	-0.53834800	-1.78792000
H	-4.47306400	-0.26841100	-2.70487200
K	-0.32573700	0.26275300	-0.07204200



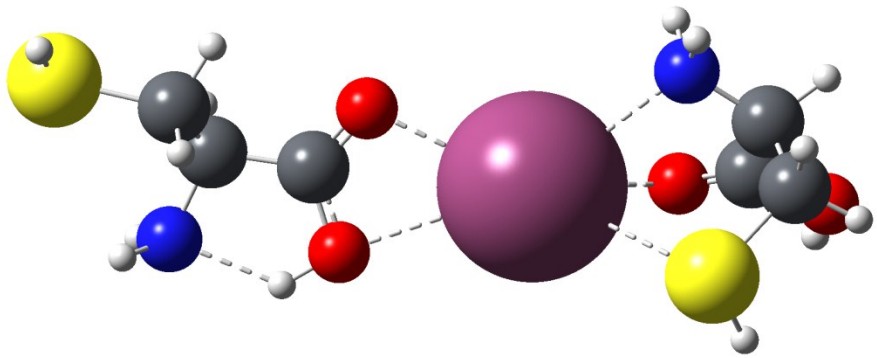
Iso_10 (8.12 kJ/mol)

H	-1.94846200	2.58545400	0.52227000
S	-2.52529600	1.99296800	-0.54208400
C	-3.88872800	1.15190900	0.37341400
H	-4.18267700	1.78765000	1.20906300
H	-4.73193500	1.11364400	-0.31508800
C	-3.58753700	-0.27146500	0.88698000
H	-4.51166100	-0.61069000	1.37623800
N	-2.42371600	-0.29411700	1.77813300
H	-2.55681600	0.38331500	2.52441200
H	-2.35346100	-1.20170200	2.23202000
C	-3.35636700	-1.22651400	-0.28120300
O	-2.29391100	-1.72590300	-0.57905100
O	-4.48808400	-1.44576000	-0.95739700
H	-4.30454000	-2.04449500	-1.69906400
H	3.02850800	1.75508900	1.60503000
S	2.49585900	1.98381000	0.38769700
C	3.80778200	1.13602900	-0.59554900
H	3.87898500	1.69345700	-1.53117200
H	4.75697500	1.25035700	-0.07592400
C	3.55365300	-0.34898200	-0.92258600
H	4.47149700	-0.71417800	-1.40501500
N	2.36185000	-0.50659000	-1.76192600
H	2.45759900	0.06532800	-2.59679200
H	2.28894400	-1.46840700	-2.08471800
C	3.38437800	-1.16379600	0.35532800
O	2.34582600	-1.65511300	0.73699600
O	4.53674400	-1.25772600	1.02757500
H	4.39218900	-1.77937300	1.83342500
K	-0.00341000	-0.41189600	0.00204100



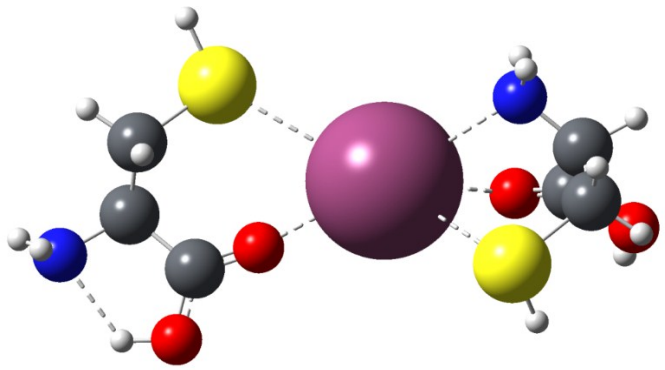
Iso_11 (8.38 kJ/mol)

H	-6.73782800	1.91753600	-0.69989100
S	-6.45168400	0.60425100	-0.60553400
C	-4.64560400	0.82030400	-0.30418500
H	-4.16736100	1.26029800	-1.17755200
H	-4.49306200	1.47891400	0.55480900
C	-4.01459700	-0.55155700	-0.03187600
H	-4.17988000	-1.19052500	-0.90588500
N	-4.50521300	-1.21249100	1.18895400
H	-5.18508100	-0.64169000	1.68223500
H	-4.94865300	-2.10265500	0.99292300
C	-2.48804400	-0.39541300	0.09004200
O	-1.77765300	0.10729500	-0.75520500
O	-1.98192200	-0.87713900	1.22586300
H	-2.77951900	-1.22361400	1.72076800
H	4.12231800	0.28284800	2.27176800
S	3.53945200	1.30120300	1.60733800
C	4.64601400	1.27360600	0.13013400
H	4.71731600	2.31144900	-0.20013700
H	5.64006600	0.96503300	0.44765600
C	4.17215200	0.40945700	-1.05593000
H	4.98495300	0.43738100	-1.79510500
N	2.89560200	0.89959800	-1.58727400
H	2.98178100	1.88567400	-1.81914700
H	2.67630000	0.42414000	-2.45948900
C	4.01850300	-1.04849000	-0.63537100
O	2.96266900	-1.62753700	-0.50279500
O	5.20550800	-1.61648000	-0.40520600
H	5.07042700	-2.53899200	-0.13408400
K	0.77694000	-0.13154600	0.13802000



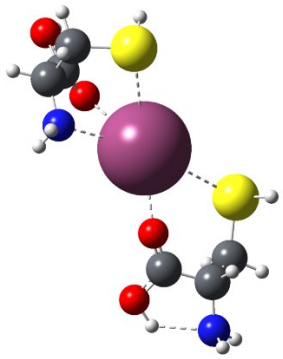
Iso_12 (9.37 kJ/mol)

H	3.13765900	3.25151700	-0.64638900
S	2.65943600	2.10634600	-0.12072000
C	4.04785500	1.01668700	-0.68077700
H	3.83389800	0.63585300	-1.68167900
H	4.94144000	1.63746100	-0.72585700
C	4.31936300	-0.14281000	0.29245300
H	4.39435300	0.26536200	1.30631900
N	5.55405900	-0.88534700	0.01613800
H	5.77316400	-0.93036800	-0.97482900
H	6.35720900	-0.50412700	0.50201600
C	3.15153500	-1.14839400	0.35069000
O	1.98628300	-0.80550800	0.30275900
O	3.51179200	-2.40876900	0.48535200
H	4.49929900	-2.41027600	0.45406500
H	-3.15388900	-2.42370200	-0.55297700
S	-2.82934800	-1.50452300	-1.48462000
C	-4.23263900	-0.34957500	-1.16526100
H	-4.46787000	0.09897500	-2.13212800
H	-5.09910600	-0.93188300	-0.85820700
C	-3.96207300	0.77884900	-0.15016900
H	-4.91962600	1.30174400	-0.01565600
N	-2.88733300	1.66198200	-0.61690600
H	-3.11660600	2.01158500	-1.54352300
H	-2.82491000	2.47903000	-0.01431000
C	-3.58825800	0.20657300	1.21298200
O	-2.48930800	0.27153800	1.71742200
O	-4.63009100	-0.40132100	1.78865500
H	-4.35457800	-0.75659100	2.64923400
K	-0.33647500	0.30496400	0.03219600



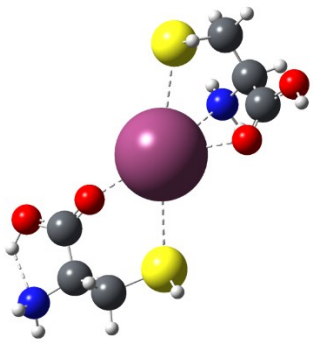
Iso_13 (11.41 kJ/mol)

H	-3.03288000	2.80120700	-0.58802200
S	-2.69230600	2.13286500	0.53303400
C	-4.14976400	1.01754000	0.57940300
H	-4.15403700	0.59586000	1.58706800
H	-5.04027200	1.64067000	0.48474700
C	-4.22363700	-0.11108500	-0.47595400
H	-4.06548000	0.31912600	-1.46909800
N	-5.51640000	-0.80269900	-0.35677000
H	-6.22292300	-0.24877400	0.11454300
H	-5.88943800	-1.08184600	-1.25804800
C	-3.10451400	-1.14678200	-0.24349300
O	-1.94051400	-0.93621200	-0.51811600
O	-3.50654600	-2.27584700	0.31091800
H	-4.49184700	-2.20517500	0.37049200
H	3.87294600	2.09524400	-0.70458300
S	3.38201800	1.19772100	-1.58297000
C	4.36112500	-0.25333700	-0.99696100
H	4.54561300	-0.85892000	-1.88603300
H	5.32570200	0.10144700	-0.63938500
C	3.68691600	-1.13752700	0.07142900
H	4.43942100	-1.88180700	0.36822500
N	2.45473900	-1.73895400	-0.44703300
H	2.65813900	-2.24796600	-1.30299800
H	2.09479800	-2.42560300	0.21148300
C	3.36560700	-0.32487200	1.32115200
O	2.25288900	-0.00865600	1.67971200
O	4.47815400	0.02193500	1.97603500
H	4.23635300	0.54103200	2.76004000
K	0.32809900	0.24654300	-0.24971900



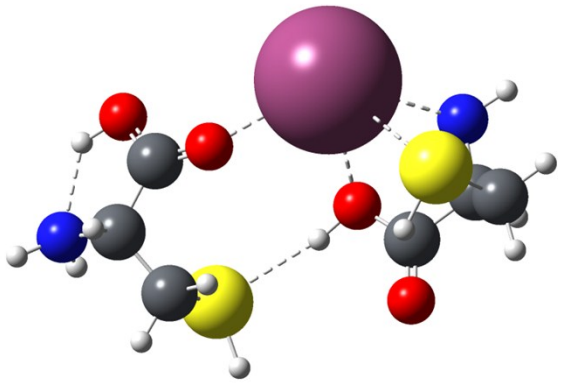
Iso_14 (12.28 kJ/mol)

H	-2.59901800	2.67553400	-0.81599400
S	-2.43072600	2.07772000	0.38129100
C	-4.04319300	1.20154900	0.42512900
H	-4.16852000	0.88700500	1.46369200
H	-4.82137400	1.93608100	0.21243200
C	-4.22986300	-0.00445400	-0.52543000
H	-3.97151100	0.30080100	-1.54367800
N	-5.61005600	-0.49844400	-0.40995000
H	-6.25478600	0.19993400	-0.05668600
H	-5.97329000	-0.83810800	-1.29444300
C	-3.27698700	-1.15261500	-0.13665900
O	-2.08815600	-1.13632300	-0.38307800
O	-3.84942000	-2.14493500	0.52017500
H	-4.81619600	-1.93660200	0.52752900
H	3.77558400	-1.84559200	-1.46826300
S	3.24324100	-2.08497700	-0.25272800
C	4.30032900	-0.90492800	0.69369100
H	4.43975900	-1.35962300	1.67610300
H	5.27743200	-0.85528800	0.21737300
C	3.72736000	0.51401500	0.88340700
H	4.52046000	1.09886700	1.37047200
N	2.48200700	0.48053700	1.65835500
H	2.64430600	-0.00498200	2.53665100
H	2.20236500	1.42654100	1.90636600
C	3.46746600	1.17823300	-0.46446500
O	2.37301900	1.41406700	-0.92664400
O	4.61133800	1.45858700	-1.09665700
H	4.40915100	1.87352200	-1.95074000
K	0.32562200	-0.26518900	-0.19689800



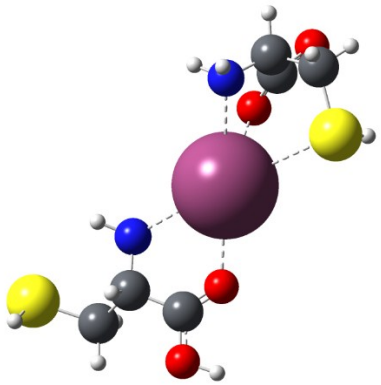
Iso_15 (12.43 kJ/mol)

H	2.00148700	3.17603200	0.04089700
S	2.26121300	1.96026800	-0.47873400
C	2.70066700	1.12388700	1.11706700
H	3.32310700	1.80346600	1.69773200
H	1.79091300	0.90252100	1.67214000
C	3.47642000	-0.17353400	0.85009200
H	3.67250900	-0.62821300	1.82775200
N	4.75060100	-0.03853200	0.14077600
H	4.77381200	0.78298700	-0.45743900
H	5.54743600	-0.00639300	0.76511100
C	2.60699500	-1.21466200	0.10899300
O	1.43102700	-1.39652800	0.36402300
O	3.24842900	-1.90587500	-0.81054800
H	4.16725000	-1.53042800	-0.82478800
H	-2.43605600	0.28339400	2.34422700
S	-3.16929500	-0.62960300	1.67603200
C	-3.94455500	0.54540700	0.47970700
H	-4.92077700	0.12043700	0.24029500
H	-4.11064500	1.48960500	0.99376600
C	-3.15695000	0.78714300	-0.81596100
H	-3.69359500	1.58309200	-1.35376300
N	-3.04778100	-0.44625900	-1.61402000
H	-3.98195500	-0.80098900	-1.80447500
H	-2.64149600	-0.22976400	-2.52098500
C	-1.79191200	1.39577400	-0.48973400
O	-1.65873800	2.38100300	0.18610300
O	-0.75767300	0.71736400	-1.03570800
H	0.08476600	1.18931800	-0.83070900
K	-0.96923800	-2.06231300	-0.40872500



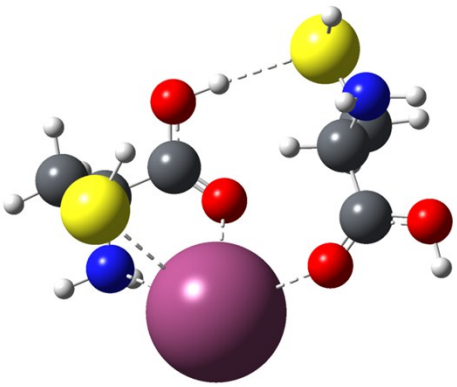
Iso_16 (12.93 kJ/mol)

K	-0.46924900	0.29669600	0.24029600
H	5.90756900	-1.18198200	1.38461800
S	5.37871400	-1.73187800	0.27188000
C	4.66229100	-0.18369300	-0.41016100
H	5.39268000	0.61951900	-0.33634700
H	4.50076400	-0.38709300	-1.47212600
C	3.32623000	0.21691400	0.25966600
H	3.52809000	0.40886500	1.32024300
N	2.26733700	-0.79634000	0.18852000
H	2.18375000	-1.12205500	-0.77416900
H	2.58028700	-1.60880300	0.71573000
C	2.79481200	1.54177700	-0.28797800
O	1.64513400	1.74718400	-0.61620500
O	3.74403700	2.48011200	-0.34158200
H	3.35418200	3.30541600	-0.67241400
H	-3.92053700	1.89880500	-0.98303300
S	-3.55886900	1.81876100	0.31342400
C	-4.57268900	0.33757000	0.74231600
H	-4.87598300	0.48053500	1.78100300
H	-5.47621700	0.34814200	0.13604500
C	-3.86325200	-1.02556800	0.61822200
H	-4.63228400	-1.78642800	0.81352600
N	-2.72427000	-1.11307600	1.53914000
H	-3.04105400	-0.91799900	2.48525000
H	-2.36355700	-2.06402700	1.55333900
C	-3.37946700	-1.25976000	-0.80889100
O	-2.21961600	-1.27711700	-1.15789900
O	-4.40527200	-1.43074900	-1.64801000
H	-4.06276300	-1.57323700	-2.54522800



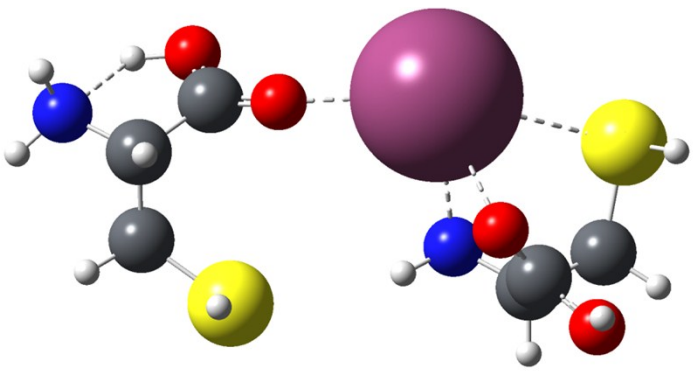
Iso_17 (14.06 kJ/mol)

K	-1.13728200	-2.21114100	-0.70534900
H	2.74211400	2.62596600	0.86029400
S	2.19533600	2.59290800	-0.37514300
C	2.63149200	0.83885000	-0.70882800
H	1.99857700	0.53730500	-1.54298700
H	3.67574500	0.78880100	-1.02169100
C	2.39478700	-0.07221100	0.51241300
H	1.36900700	0.07313200	0.85447000
N	3.29530200	0.29260000	1.59214700
H	3.05127400	-0.14790900	2.47163100
H	4.26228000	0.06900000	1.37922700
C	2.46160000	-1.53201900	0.05068300
O	1.48539600	-2.21473900	-0.20248300
O	3.71127000	-1.98492600	-0.06696500
H	3.69534700	-2.90530900	-0.37534300
H	-1.62764300	0.23314900	2.43896700
S	-2.59464000	-0.51561000	1.87243500
C	-3.37941500	0.83886900	0.88912100
H	-4.45114300	0.63419400	0.90684700
H	-3.21595000	1.77896400	1.41131700
C	-2.91121500	0.95066400	-0.57200000
H	-3.38081700	1.85937400	-0.97588800
N	-3.26255500	-0.25842400	-1.32960300
H	-4.26429200	-0.41887700	-1.26221000
H	-3.06714100	-0.11202300	-2.31706000
C	-1.40254200	1.17356800	-0.65280100
O	-0.63456800	0.38437400	-1.17393700
O	-1.03010800	2.30497500	-0.08045200
H	-0.04352700	2.41612200	-0.14128700



Iso_18 (14.74 kJ/mol)

H	-2.30799800	2.58289500	-0.91537800
S	-2.12499400	2.16224200	0.35282600
C	-3.72200500	1.28507100	0.53863800
H	-3.75748000	0.98219400	1.58773700
H	-4.52464700	2.00777100	0.38102000
C	-3.98848300	0.06479400	-0.37367400
H	-3.88994900	0.37221900	-1.41913300
N	-5.31732700	-0.47406300	-0.04631600
H	-5.94634500	0.23043200	0.32351700
H	-5.76860200	-0.89918800	-0.85014400
C	-2.95843400	-1.05183300	-0.13005900
O	-1.85522000	-1.06623900	-0.63621200
O	-3.36220900	-1.99914700	0.70254400
H	-4.31550000	-1.80899100	0.88170200
H	4.68966000	-1.34291700	-0.39978200
S	3.82752700	-1.61451800	0.60078400
C	3.77244800	0.08368900	1.32211200
H	3.62977600	-0.05998800	2.39456900
H	4.74443600	0.55288300	1.18289400
C	2.65068900	1.00256300	0.79494500
H	2.81929600	1.98578600	1.25693800
N	1.33321000	0.43880100	1.09585400
H	1.24637400	0.29280900	2.09772500
H	0.58976600	1.08379000	0.83377400
C	2.78602600	1.20246600	-0.70994100
O	2.04650700	0.73056900	-1.54555600
O	3.84971800	1.95496700	-1.00879900
H	3.91116800	2.04872800	-1.97314600
K	0.67665900	-1.52773000	-0.88077600



Iso 19 (17.67 kJ/mol)

K	-1.03596900	-2.11325200	0.42909700
H	4.44047700	2.43287700	-0.12434600
S	3.11136400	2.51483700	0.09367100
C	2.85826900	0.76867700	0.59975100
H	3.58754700	0.50426000	1.36442900
H	1.86246600	0.74719800	1.04675700
C	2.92040700	-0.23660200	-0.57475300
H	3.94710000	-0.24579800	-0.96070300
N	1.92683600	0.10469200	-1.59353300
H	2.09342100	1.07263800	-1.86588900
H	2.07133800	-0.45965500	-2.42693700
C	2.65939000	-1.62512400	-0.00031100
O	1.57885100	-2.17252400	0.08827900
O	3.78941500	-2.17495100	0.45373200
H	3.58939600	-3.03456100	0.85772000
H	-4.43638700	-0.03502700	1.17650800
S	-4.14021500	-0.63826600	0.00756000
C	-3.52836700	0.86180600	-0.87817200
H	-3.80777300	0.71711700	-1.92306300
H	-4.07308100	1.72948500	-0.51100300
C	-2.00564900	1.10348400	-0.80562500
H	-1.82669800	2.06952300	-1.30028900
N	-1.27135400	-0.00535100	-1.41342600
H	-1.54891200	-0.09884100	-2.38638900
H	-0.25878300	0.15843300	-1.40623200
C	-1.56435800	1.27832100	0.64155300
O	-0.90309600	0.48033300	1.27229000
O	-2.01448800	2.42638300	1.15576700
H	-1.72707400	2.49631300	2.08041500

Iso 20 (19.17 kJ/mol)

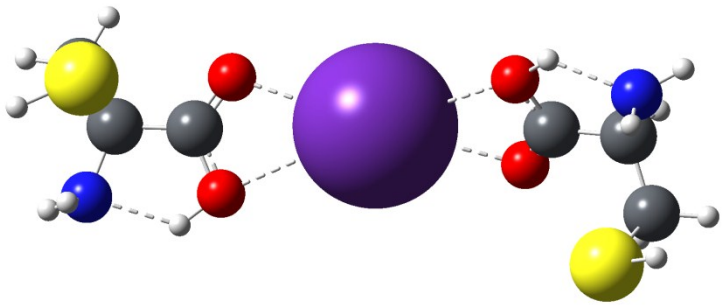
H	-3.23790300	-1.34142500	-1.72817500
S	-2.35078500	-1.78152900	-0.80944900
C	-3.40949400	-1.38450700	0.64733400
H	-4.10387000	-2.21234700	0.79771400
H	-2.74901700	-1.34533900	1.51314700
C	-4.21258700	-0.08573300	0.52823100
H	-4.78593000	0.00849800	1.46861200
N	-5.06955200	-0.11391800	-0.65672900
H	-5.80388700	-0.80659400	-0.54876500
H	-5.51440900	0.78303500	-0.81762900
C	-3.33271000	1.16064500	0.51347400
O	-2.15429200	1.20179200	0.80016700
O	-4.03599700	2.25166300	0.19160900
H	-3.46046900	3.03141400	0.23874500
H	3.57193600	2.25786400	0.73106200
S	3.11521600	2.02451700	-0.51596100
C	4.22244200	0.59899200	-0.90205700
H	4.41817600	0.66319500	-1.97387500
H	5.17057200	0.74786300	-0.38920000
C	3.65782000	-0.80061800	-0.58609000
H	4.47402500	-1.50921300	-0.78573800
N	2.45393300	-1.07279100	-1.37851400
H	2.66493500	-0.95289300	-2.36570300
H	2.17521400	-2.04465000	-1.26598200
C	3.32698000	-0.92923000	0.89694800
O	2.20859700	-0.98694400	1.35873400
O	4.43529500	-0.95133200	1.64290800
H	4.18795200	-1.02818300	2.57865000
K	0.20671500	0.24680000	-0.02810500

Atomic Coordinates $[(Cys)_2Rb]^+$

Note: Energies include thermal correction at 298 K

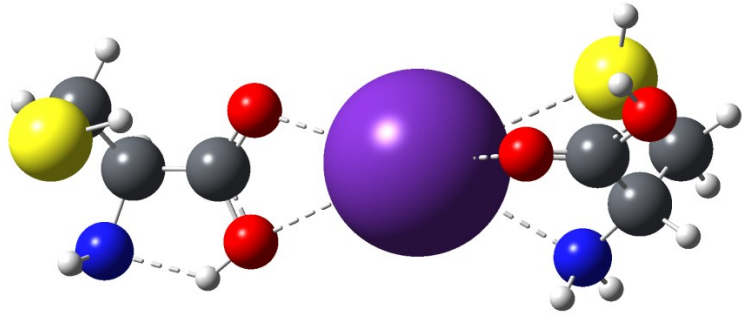
Iso_1 (GM)

H	6.29275700	0.71655100	-2.30728600
S	5.19236100	1.22346000	-1.71633900
C	5.62762400	0.77914300	0.01970500
H	6.71182200	0.74922500	0.11939800
H	5.25142500	1.58898300	0.64353800
C	5.01204600	-0.54808500	0.48907700
H	5.35236000	-0.72362300	1.51705600
N	5.32635200	-1.74022900	-0.30347800
H	5.47185000	-1.50427900	-1.28212200
H	6.14013000	-2.23721200	0.03851900
C	3.48145900	-0.43818800	0.60160800
O	2.89200200	0.52755000	1.03422300
O	2.82364000	-1.53277600	0.20788300
H	3.53132300	-2.14883200	-0.12078800
H	-6.29040300	-0.74016100	-2.30191700
S	-5.18988300	-1.24022500	-1.70540100
C	-5.62701000	-0.78019800	0.02606900
H	-6.71131400	-0.75021400	0.12457300
H	-5.25070000	-1.58393200	0.65768300
C	-5.01283700	0.55179500	0.48364000
H	-5.35384900	0.73644700	1.50978700
N	-5.32769500	1.73637600	-0.31996600
H	-5.47252400	1.49138700	-1.29648700
H	-6.14202400	2.23583700	0.01707400
C	-3.48221600	0.44418600	0.59790900
O	-2.89220900	-0.51710400	1.03959500
O	-2.82508300	1.53561100	0.19441800
H	-3.53309900	2.14808000	-0.14018500
Rb	-0.00024900	0.00429200	0.77881400



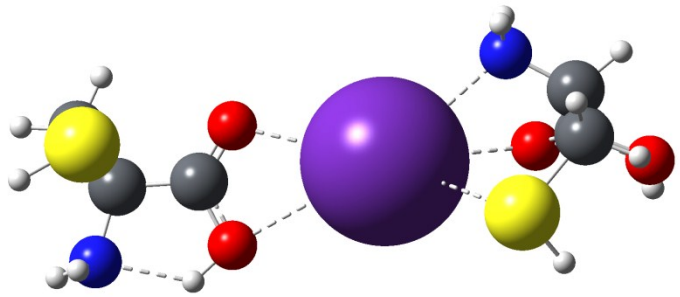
Iso_2 (3.98 kJ/mol)

H	-4.13159000	2.13861900	-0.43259500
S	-5.40014400	1.72758700	-0.22991000
C	-5.22287200	0.08142100	-1.03109400
H	-6.24353900	-0.25099000	-1.22464900
H	-4.71494000	0.19306200	-1.98764100
C	-4.50578100	-0.96633200	-0.16489700
H	-4.55875900	-1.92451400	-0.69658500
N	-5.03721100	-1.16065100	1.18821300
H	-5.46371000	-0.30274800	1.53409400
H	-5.72052700	-1.90707700	1.23656400
C	-2.99998400	-0.67455600	-0.04752300
O	-2.29979400	-0.28596100	-0.95696700
O	-2.49350600	-0.92384200	1.16353700
H	-3.28361000	-1.18755200	1.71139300
H	4.02787100	-0.37517800	-2.34816800
S	3.66596100	-1.33344200	-1.47168800
C	4.86255200	-0.88454600	-0.14062400
H	5.14069900	-1.82703000	0.33433100
H	5.75792200	-0.47824100	-0.60640300
C	4.34185600	0.07983500	0.94250900
H	5.21269900	0.33001700	1.56636400
N	3.24619000	-0.52395900	1.70734200
H	3.55933100	-1.40697200	2.10166900
H	3.01001200	0.07048500	2.49796200
C	3.87058900	1.39363900	0.32872600
O	2.72896000	1.79477700	0.32741500
O	4.88903800	2.06152200	-0.22635000
H	4.55636400	2.89453000	-0.59729000
Rb	0.49892200	-0.15754600	0.05632400



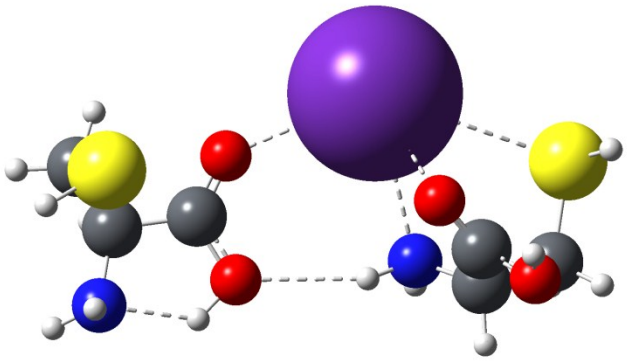
Iso_3 (5.61 kJ/mol)

H	-6.11695600	2.02371800	0.22197100
S	-4.91740500	1.88299700	-0.37657200
C	-5.14923400	0.15294800	-0.97191400
H	-6.21091300	-0.02938900	-1.13297600
H	-4.64427500	0.09336800	-1.93521700
C	-4.56276100	-0.90763200	-0.02761300
H	-4.77786100	-1.89123600	-0.46312200
N	-5.05209400	-0.90654300	1.35393800
H	-5.30267500	0.03228600	1.65475300
H	-5.84841900	-1.51776500	1.48988900
C	-3.02609500	-0.82795700	0.00757100
O	-2.32778700	-0.62319900	-0.96031800
O	-2.49507500	-1.04279700	1.21501700
H	-3.27646400	-1.15208400	1.81909000
H	3.83179500	0.78437300	2.33757500
S	3.18139700	1.59799500	1.48165600
C	4.43293300	1.54396400	0.12662400
H	4.39982600	2.52891900	-0.34239800
H	5.41818800	1.42933000	0.57372300
C	4.21283000	0.47227800	-0.95869200
H	5.10824500	0.50256600	-1.59701700
N	2.97280600	0.71713800	-1.70071900
H	2.99221400	1.65659400	-2.08826100
H	2.91459000	0.08474200	-2.49498300
C	4.17483300	-0.92509600	-0.34954800
O	3.20818300	-1.65240500	-0.32635000
O	5.36094900	-1.25628300	0.17582100
H	5.30370800	-2.15213000	0.54495200
Rb	0.48851200	-0.46532100	-0.04415700



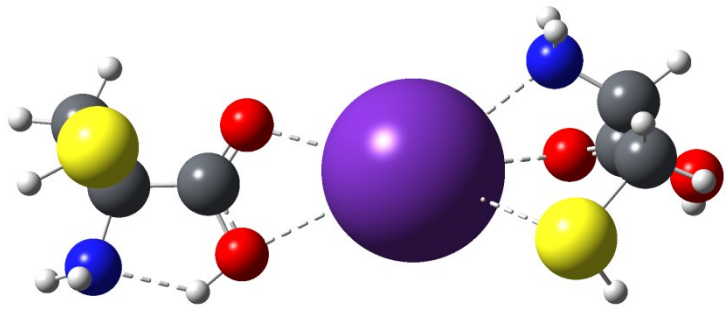
Iso_4 (5.61 kJ/mol)

H	5.59597500	0.70777400	1.78906700
S	4.43573700	0.02988400	1.68785700
C	4.65934200	-0.56969600	-0.04307700
H	5.72292700	-0.59069500	-0.27649100
H	4.28719200	-1.59294400	-0.06676700
C	3.90295500	0.26914900	-1.08380100
H	4.12246300	-0.15580400	-2.07116900
N	4.21382800	1.70040400	-1.12832100
H	4.46250800	2.05068800	-0.20600400
H	4.96065500	1.92159100	-1.77608600
C	2.37651600	0.11348900	-0.92895900
O	1.82762100	-0.93495300	-0.66546100
O	1.69651300	1.23496500	-1.15305200
H	2.39795900	1.92290500	-1.30873400
H	-4.92611500	-0.56665600	0.72544600
S	-4.35644100	-0.72828600	-0.48566200
C	-4.03299500	1.05732800	-0.82352600
H	-4.15079900	1.17628500	-1.90198600
H	-4.81190000	1.64580300	-0.34293100
C	-2.63810600	1.57759900	-0.42048600
H	-2.66326700	2.66542600	-0.58420100
N	-1.58990600	0.90077900	-1.18246700
H	-1.74635400	1.04655700	-2.17566300
H	-0.67150600	1.28913100	-0.97663900
C	-2.40191200	1.38052000	1.07230300
O	-1.60292000	0.61585400	1.56286000
O	-3.21371700	2.16166400	1.79801800
H	-3.03720000	2.00776600	2.73982200
Rb	-0.81171600	-1.84195300	0.11889400



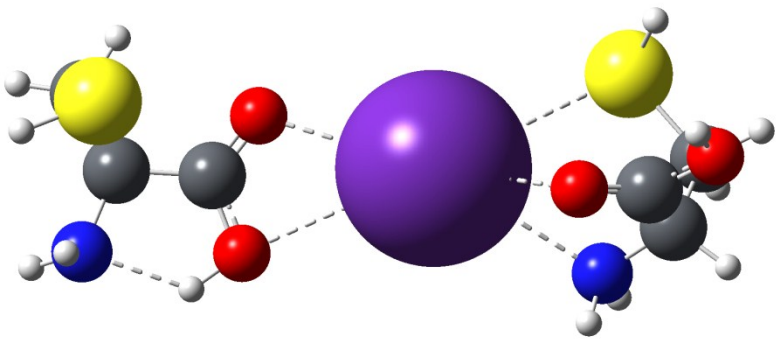
Iso_5 (5.61 kJmol)

H	6.13363200	2.01062400	-0.21507600
S	4.93131300	1.87608100	0.37931000
C	5.15222600	0.14493900	0.97560600
H	6.21241000	-0.04287300	1.14018200
H	4.64378700	0.08802800	1.93723700
C	4.56346400	-0.91270400	0.02941700
H	4.77198600	-1.89734700	0.46577500
N	5.05750600	-0.91432300	-1.35043300
H	5.31372500	0.02319700	-1.65058400
H	5.85126400	-1.52949200	-1.48355800
C	3.02735600	-0.82510400	-0.01101600
O	2.32688300	-0.61666800	0.95456800
O	2.49932000	-1.03727900	-1.22011600
H	3.28207500	-1.15086700	-1.82156600
H	-3.85258700	0.75975300	-2.33820100
S	-3.20539700	1.58496100	-1.49098400
C	-4.45032400	1.52978500	-0.12991900
H	-4.42360900	2.51827800	0.33200500
H	-5.43654600	1.40349300	-0.57171000
C	-4.21610500	0.46774400	0.96188500
H	-5.10887800	0.49476200	1.60404500
N	-2.97494900	0.72858400	1.69660100
H	-3.00107600	1.67038900	2.07801300
H	-2.90757900	0.10205800	2.49479300
C	-4.16860000	-0.93349400	0.36243500
O	-3.19582800	-1.65264100	0.34053300
O	-5.35385300	-1.27851700	-0.15589100
H	-5.29038900	-2.17645200	-0.51887200
Rb	-0.48759600	-0.44584400	0.03859300



Iso_6 (6.10 kJ/mol)

H	-6.26679300	1.91758200	0.03708000
S	-5.03756200	1.81224800	-0.50592200
C	-5.16080200	0.04990000	-1.03529300
H	-6.20486700	-0.19155700	-1.23017400
H	-4.61398200	-0.02386700	-1.97445600
C	-4.56369200	-0.94058900	-0.02388500
H	-4.71333200	-1.95065900	-0.42486700
N	-5.10943600	-0.90703600	1.33595500
H	-5.41573900	0.03018100	1.58602200
H	-5.88165300	-1.54968500	1.46591100
C	-3.03527500	-0.78351400	0.06826100
O	-2.30958300	-0.58348200	-0.88066000
O	-2.54430900	-0.92207400	1.30237800
H	-3.34328000	-1.04508700	1.87994000
H	3.99219000	0.21851100	-2.39293600
S	3.63994600	-0.92782500	-1.77698900
C	4.84334500	-0.81249300	-0.38305600
H	5.12699700	-1.84124800	-0.15401100
H	5.73480000	-0.30095700	-0.73995000
C	4.32646400	-0.14399100	0.90556600
H	5.20065600	-0.04817900	1.56649300
N	3.23862300	-0.92192600	1.50652000
H	3.55789400	-1.87253000	1.67267800
H	3.00426800	-0.53861600	2.41883300
C	3.84543800	1.27691000	0.63272600
O	2.70239000	1.65997100	0.73602000
O	4.85718300	2.06569700	0.25032900
H	4.51783900	2.96169300	0.09483800
Rb	0.47525000	-0.18248300	0.01549700

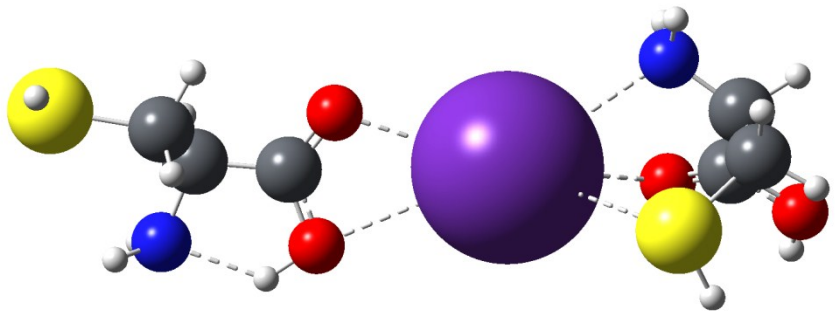


Iso_7 (8.81 kJ/mol)

Rb	-1.91758400	1.90123300	-0.40233000
H	-1.88661900	-1.90153700	-2.05073300
S	-3.00533300	-1.33976300	-1.55285300
C	-3.03375700	-2.28772900	0.03502600
H	-4.08555700	-2.50183600	0.23125300
H	-2.52932300	-3.23567600	-0.13511400
C	-2.42764500	-1.56805500	1.24639900
H	-2.39370300	-2.31300400	2.05862600
N	-3.21287600	-0.37869100	1.60191500
H	-4.16491900	-0.65119200	1.82954300
H	-2.82202300	0.04647800	2.43813600
C	-0.97795700	-1.14039200	1.01527000
O	-0.57004300	-0.03620600	1.34168500
O	-0.23872500	-2.05925400	0.43411800
H	0.66417100	-1.66108000	0.15294000
H	5.40136900	-1.41961900	0.95804200
S	5.22780800	-1.26319600	-0.37120400
C	4.20715800	0.25832400	-0.27619900
H	4.70071800	0.99356000	0.35772200
H	4.18952200	0.64839400	-1.29687900
C	2.75914000	-0.00000700	0.22122400
H	2.80892600	-0.33038000	1.26233800
N	2.03302600	-1.01190600	-0.55381400
H	1.76540500	-0.62311500	-1.45676400
H	2.67464000	-1.78469500	-0.73796600
C	1.99619200	1.31582800	0.21051900
O	1.13027700	1.62629400	-0.57989100
O	2.45089400	2.13282600	1.16831200
H	2.00935400	2.99251800	1.09605300

Iso_8 (12.82 kJ/mol)

H	-7.01304800	2.14548800	-0.20516100
S	-6.79044600	0.83666000	-0.43483100
C	-4.96800900	0.89627800	-0.15600800
H	-4.48034500	1.43457000	-0.96677200
H	-4.76157900	1.40695600	0.78784100
C	-4.41512400	-0.53544500	-0.10851600
H	-4.63208000	-1.02532500	-1.06358500
N	-4.92388200	-1.32181500	1.02691000
H	-5.66410700	-0.83270900	1.52141800
H	-5.30226900	-2.21579300	0.73397200
C	-2.88027300	-0.46940900	0.00012700
O	-2.15910200	0.04732700	-0.82574100
O	-2.38943000	-1.03587300	1.10312400
H	-3.19656000	-1.37877400	1.58146800
H	4.10904900	0.63436300	2.34532700
S	3.53004800	1.52592600	1.51622600
C	4.77879900	1.41675000	0.16184300
H	4.82998200	2.41724700	-0.27125800
H	5.74899400	1.20431800	0.60606500
C	4.47510900	0.40684500	-0.96184000
H	5.37243000	0.38596700	-1.59782000
N	3.26249200	0.78029700	-1.69583800
H	3.36144800	1.72830200	-2.04894800
H	3.15616100	0.18428000	-2.51295300
C	4.31911300	-1.00370400	-0.40400200
O	3.29545500	-1.64889400	-0.40916000
O	5.47110500	-1.45042400	0.11110200
H	5.33879900	-2.35132300	0.44723500
Rb	0.68452200	-0.25171100	-0.08110500



Iso_9 (12.84 kJ/mol)

H	-3.38869500	-2.31743500	0.77352300
S	-2.91318100	-2.04011400	-0.45700200
C	-4.22033600	-0.82821200	-0.93398200
H	-4.37289500	-0.96552700	-2.00591700
H	-5.14604400	-1.10653500	-0.43476900
C	-3.89567800	0.65412100	-0.66730700
H	-4.82080300	1.20907000	-0.88432800
N	-2.75770400	1.09922600	-1.47568800
H	-2.95595900	0.93195600	-2.45834000
H	-2.63430900	2.10365200	-1.37723800
C	-3.59680900	0.89566200	0.80807000
O	-2.53400000	1.26025600	1.25643300
O	-4.67243600	0.64742600	1.56684700
H	-4.45048500	0.82340600	2.49506100
H	3.38869000	-2.31743500	-0.77352500
S	2.91317900	-2.04011500	0.45700000
C	4.22033600	-0.82821400	0.93397900
H	4.37289700	-0.96552900	2.00591400
H	5.14604400	-1.10653800	0.43476500
C	3.89568000	0.65411900	0.66730500
H	4.82080600	1.20906700	0.88432300
N	2.75770900	1.09922600	1.47568800
H	2.95596600	0.93195700	2.45834000
H	2.63431400	2.10365200	1.37723700
C	3.59680700	0.89566000	-0.80807100
O	2.53400000	1.26026100	-1.25643100
O	4.67243300	0.64742600	-1.56685200
H	4.45048000	0.82341100	-2.49506400
Rb	0.00000000	0.25285400	0.00000300

Iso_10 (13.01 kJ/mol)

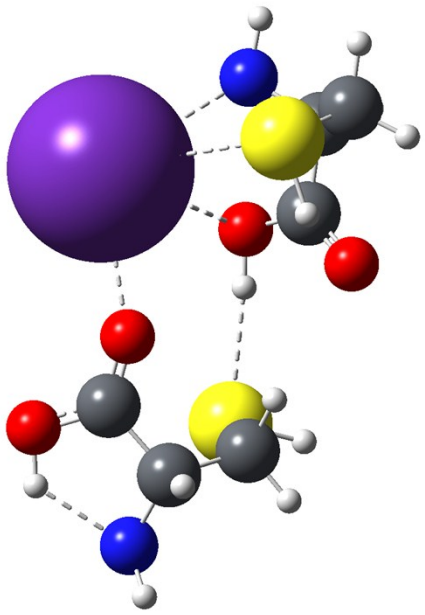
H	-3.61898800	-2.31367500	0.51028600
S	-3.10265400	-1.93040700	-0.67449500
C	-4.28385000	-0.54998600	-0.99780400
H	-4.42890200	-0.53362900	-2.07939600
H	-5.23992800	-0.80312600	-0.54449600
C	-3.82990700	0.84870600	-0.53844600
H	-4.69717200	1.51011500	-0.68453300
N	-2.64346000	1.28893800	-1.27740600
H	-2.84447800	1.27892600	-2.27361300
H	-2.42711000	2.25380400	-1.04051100
C	-3.53272700	0.86896300	0.95671100
O	-2.44863700	1.07799300	1.45068300
O	-4.63611500	0.61919300	1.67385800
H	-4.41257300	0.65358600	2.61768500
H	3.61703300	2.31376500	0.50959800
S	3.10120900	1.93037000	-0.67536700
C	4.28303900	0.55042700	-0.99841700
H	4.42772800	0.53369800	-2.08005300
H	5.23912100	0.80434200	-0.54555400
C	3.83012400	-0.84832600	-0.53827500
H	4.69785300	-1.50918600	-0.68415400
N	2.64389700	-1.28984900	-1.27680900
H	2.84453700	-1.27971500	-2.27308700
H	2.42859100	-2.25490100	-1.03973600
C	3.53324700	-0.86813600	0.95696700
O	2.44962200	-1.07872700	1.45129800
O	4.63640300	-0.61625200	1.67375200
H	4.41316800	-0.65072700	2.61764800
Rb	0.00030900	-0.00064500	0.09259600

Iso_11 (14.16 kJ/mol)

H	-3.52276200	3.24813300	0.57816800
S	-3.00210400	2.08573300	0.13717500
C	-4.38339700	1.00029600	0.72249100
H	-4.15103100	0.62244300	1.72043200
H	-5.27468600	1.62280700	0.78441000
C	-4.67638000	-0.16271700	-0.23955100
H	-4.77304900	0.24147900	-1.25307600
N	-5.90557100	-0.90422900	0.06524200
H	-6.09870000	-0.95166600	1.06152500
H	-6.71987000	-0.51769000	-0.39734700
C	-3.50954700	-1.16792700	-0.31843000
O	-2.34442900	-0.82677600	-0.28786100
O	-3.87427700	-2.42952300	-0.45175600
H	-4.86046700	-2.43053600	-0.40207600
H	3.58362800	-2.40645500	0.74789800
S	3.15311500	-1.44167700	1.58531200
C	4.49502600	-0.22488300	1.23513200
H	4.66896300	0.29988600	2.17620700
H	5.40332500	-0.77387200	0.99573800
C	4.19671700	0.81461500	0.13764800
H	5.13760500	1.36204600	-0.02251200
N	3.08539600	1.68898500	0.52414100
H	3.30040600	2.13295300	1.41280600
H	2.98729800	2.44134700	-0.15283900
C	3.87206100	0.13762500	-1.18932100
O	2.80604200	0.19133100	-1.75863400
O	4.92657600	-0.54176900	-1.65780300
H	4.68774800	-0.94883400	-2.50594400
Rb	0.29401200	0.18193600	-0.14238500

Iso_12 (14.33 kJ/mol)

H	-2.64608000	-3.05227700	-1.12450700
S	-2.62655000	-1.70538900	-1.14383500
C	-2.68387700	-1.45029900	0.69326800
H	-3.27986600	-2.25132000	1.12827100
H	-1.66984700	-1.50362000	1.08600600
C	-3.32899800	-0.09943400	1.03017800
H	-3.27107500	0.01387600	2.11903100
N	-4.72688300	0.07623900	0.62901600
H	-4.95337800	-0.46140800	-0.20372800
H	-5.37999800	-0.17225000	1.36223000
C	-2.50738500	1.08749100	0.47744900
O	-1.29214500	1.10516500	0.46280400
O	-3.23686100	2.09751000	0.04183400
H	-4.17779100	1.79728000	0.13158800
H	1.76965200	-0.61645900	2.43411600
S	2.85370600	0.00669800	1.93105600
C	3.42932300	-1.39429700	0.87782800
H	4.50773600	-1.26005900	0.77750900
H	3.26165100	-2.31703700	1.42874100
C	2.79662300	-1.49616600	-0.51483700
H	3.16819200	-2.44122500	-0.94508700
N	3.13995500	-0.33880200	-1.35852100
H	4.15209500	-0.25584800	-1.41092300
H	2.82024900	-0.50749100	-2.30869600
C	1.28490900	-1.70111100	-0.41512600
O	0.76011400	-2.37975100	0.43205600
O	0.60566500	-1.07144700	-1.39311100
H	-0.34949000	-1.31304400	-1.32942700
Rb	1.21308600	2.04510700	-0.53717200

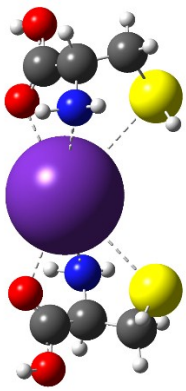


Iso_13 (15.23 kJ/mol)

H	3.18925300	2.70133400	0.84684000
S	2.97976800	2.15648600	-0.36910700
C	4.51190400	1.14955600	-0.42918400
H	4.60614700	0.83612200	-1.47138400
H	5.35220800	1.81115900	-0.21243900
C	4.59920400	-0.07891800	0.50679400
H	4.38434800	0.23712300	1.53191900
N	5.92699800	-0.69348300	0.35825300
H	6.63408000	-0.03681800	0.04644600
H	6.25434800	-1.11451400	1.22172700
C	3.54056000	-1.12995600	0.12087300
O	2.36985900	-1.03251900	0.42128200
O	4.00479900	-2.13719900	-0.60239900
H	4.98422300	-2.01248300	-0.63693000
H	-4.07640000	-1.82441000	1.43240500
S	-3.52459500	-2.04292600	0.22193300
C	-4.59275500	-0.87328700	-0.72429300
H	-4.72604000	-1.32672400	-1.70809700
H	-5.56993300	-0.83735300	-0.24729400
C	-4.03810200	0.55257000	-0.90877000
H	-4.85055200	1.13467200	-1.36862300
N	-2.81383300	0.54439700	-1.71489800
H	-3.00016100	0.08901100	-2.60429600
H	-2.54028000	1.49836800	-1.93662300
C	-3.75708000	1.21074500	0.43751500
O	-2.66369800	1.52803900	0.84705000
O	-4.88743100	1.39433600	1.13159900
H	-4.67323000	1.82248500	1.97583900
Rb	-0.30306900	-0.18261700	0.17794500

Iso_14 (16.80 kJ/mol)

H	2.06322600	2.57553100	-0.36231800
S	2.67927900	2.01426000	0.69702900
C	4.11379700	1.30901400	-0.22092700
H	4.40685300	2.01697700	-0.99688700
H	4.92924100	1.26254500	0.49953600
C	3.90634700	-0.08561800	-0.84344800
H	4.87338500	-0.35230400	-1.29588000
N	2.80195600	-0.09476700	-1.80592100
H	2.96604100	0.61688200	-2.51303900
H	2.78258000	-0.98368000	-2.29925500
C	3.65535900	-1.13552400	0.23504000
O	2.63653500	-1.77475500	0.36879300
O	4.72250400	-1.27545600	1.03042300
H	4.53193700	-1.95274200	1.69872100
H	-3.30677200	1.68834300	-1.75734800
S	-2.67934300	1.99330800	-0.60379800
C	-3.97360300	1.33532400	0.53530900
H	-3.95561300	1.98872500	1.40930400
H	-4.94370800	1.45632400	0.05785200
C	-3.78760000	-0.12122700	1.00242400
H	-4.70645200	-0.38134400	1.54881300
N	-2.57741200	-0.26562700	1.81585600
H	-2.62086400	0.37733900	2.60181300
H	-2.53898000	-1.19999100	2.21521900
C	-3.71876600	-1.07413500	-0.18593200
O	-2.75073300	-1.72506600	-0.50569600
O	-4.88015400	-1.10044900	-0.85275600
H	-4.80476400	-1.72437200	-1.59234600
Rb	-0.00663000	-0.57696700	-0.11449600

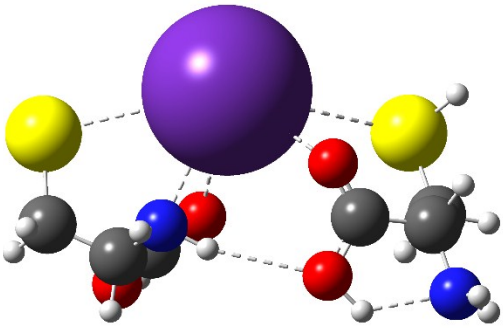


Iso_15 (17.69 kJ/mol)

H	-3.17328300	2.72289600	-0.77071300
S	-2.96870000	2.14384100	0.43016500
C	-4.50562600	1.14280300	0.45969300
H	-4.60294200	0.80051700	1.49248700
H	-5.34242000	1.81430000	0.26052700
C	-4.59715500	-0.05817500	-0.51090900
H	-4.37773100	0.28561100	-1.52608700
N	-5.92870800	-0.66929500	-0.38342600
H	-6.63292800	-0.01807700	-0.05421700
H	-6.25625700	-1.06320000	-1.25952700
C	-3.54531200	-1.12564100	-0.15232800
O	-2.37318200	-1.02577100	-0.44632100
O	-4.01712100	-2.15092100	0.53995800
H	-4.99596400	-2.02194700	0.57535800
H	4.07971500	-1.91229600	-1.31420900
S	3.52536800	-2.05208000	-0.09331400
C	4.59133300	-0.82335900	0.77754300
H	4.72357400	-1.21264600	1.78858500
H	5.56912300	-0.81720100	0.30050600
C	4.03526400	0.61084200	0.86933000
H	4.84649600	1.22203500	1.29215300
N	2.80970200	0.65332100	1.67242500
H	2.99533500	0.25724800	2.58991700
H	2.53436700	1.61928500	1.83102500
C	3.75570900	1.18137800	-0.51665600
O	2.66288000	1.47339700	-0.94601100
O	4.88647900	1.31846700	-1.22069200
H	4.67311300	1.69190900	-2.09072500
Rb	0.30293100	-0.19495300	-0.17576200

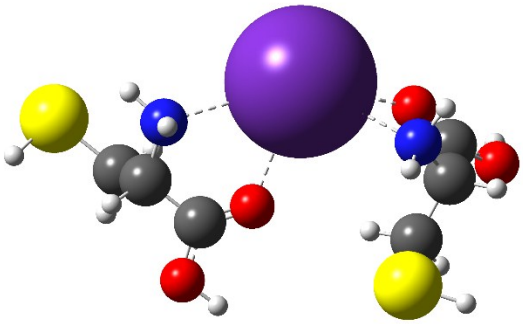
Iso 16 (18.40 kJ/mol)

H	3.93989400	-2.16629900	0.90882900
S	2.99335700	-1.41004900	1.50187900
C	3.69833000	0.22295900	1.05997100
H	3.08563200	0.94728400	1.60191200
H	4.70879200	0.27792200	1.46890700
C	3.76127500	0.60232000	-0.43865700
H	4.33887500	-0.15545900	-0.97604800
N	4.32658100	1.95622800	-0.55409900
H	4.93996600	2.19072800	0.21913200
H	4.85497300	2.07752100	-1.41249700
C	2.35413600	0.62169300	-1.05540100
O	1.76684500	-0.36833000	-1.42381600
O	1.80042400	1.83565400	-1.11533600
H	2.51635800	2.46459000	-0.85082600
H	-4.44290600	-0.68763700	1.10056100
S	-4.10169600	-0.71240100	-0.20336800
C	-3.87378900	1.10760500	-0.41202500
H	-4.19848900	1.32859700	-1.43016500
H	-4.55292500	1.61920600	0.26676100
C	-2.43412300	1.62855600	-0.23016500
H	-2.50461700	2.72679500	-0.26041400
N	-1.54588700	1.07549800	-1.24995100
H	-1.88792700	1.32881400	-2.17239000
H	-0.60952100	1.46747700	-1.17138000
C	-1.90415400	1.28081600	1.15559700
O	-0.98243300	0.53196700	1.38877800
O	-2.60025700	1.90987100	2.11332100
H	-2.23652300	1.66310900	2.97836400
Rb	-0.51810000	-1.79466300	-0.44859700



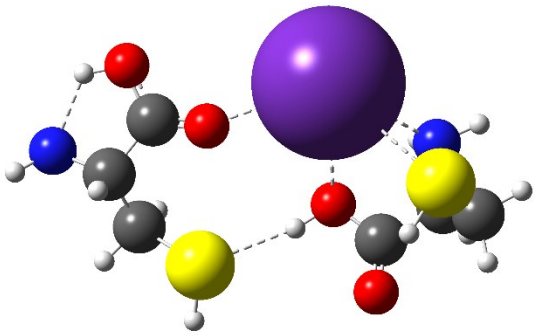
Iso 17 (22.54 kJ/mol)

Rb	-0.01049400	-1.68290500	0.66613600
H	-4.35181000	2.92978100	0.51605200
S	-3.02553500	2.70524000	0.62306200
C	-2.94621300	1.26414200	-0.51189900
H	-3.44216300	1.51201700	-1.44929100
H	-1.88004900	1.13244000	-0.70724000
C	-3.53961100	-0.03626300	0.07820600
H	-4.61991200	0.10609300	0.20091500
N	-2.85916100	-0.39414900	1.32648100
H	-2.84273000	0.43698300	1.91618400
H	-3.40573600	-1.08815300	1.83011900
C	-3.34680500	-1.14069500	-0.95962800
O	-2.41379800	-1.91338100	-0.99781400
O	-4.32714200	-1.12929300	-1.86942300
H	-4.14816400	-1.81222900	-2.53585500
H	6.13969700	0.51924200	-0.20291700
S	5.41532400	-0.56137800	-0.56143100
C	3.86331500	0.33721300	-0.95132300
H	4.07507900	1.14893800	-1.64554500
H	3.24076900	-0.39694300	-1.46769200
C	3.11922800	0.87960600	0.29135000
H	3.74117200	1.66459000	0.73783400
N	2.80646700	-0.20441300	1.22769500
H	3.64840800	-0.77113900	1.32829900
H	2.62256100	0.18498800	2.14910800
C	1.83547500	1.55119600	-0.19255900
O	0.73833200	1.03516200	-0.22268300
O	2.07504600	2.79252200	-0.62753300
H	1.25157000	3.17772300	-0.96760700



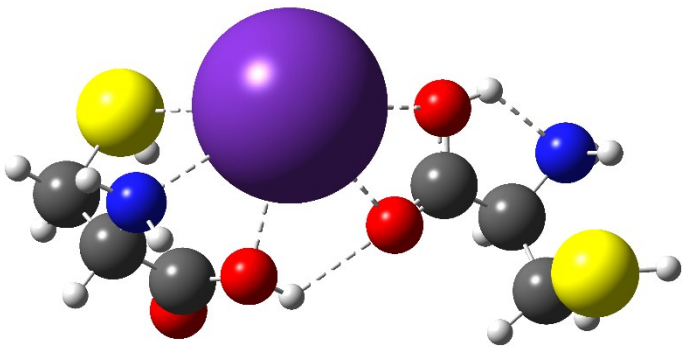
Iso 18 (22.94 kJ/mol)

H	2.02253700	3.50395400	0.31297200
S	1.87508000	2.18912100	0.57490400
C	3.40927100	1.63087100	-0.29754300
H	3.20061500	1.48783500	-1.35992900
H	4.14460000	2.42699700	-0.18967100
C	4.00083800	0.35097900	0.31685700
H	4.05018500	0.47871500	1.40375100
N	5.35140300	0.02573300	-0.15871000
H	5.51317600	0.32430800	-1.11620000
H	6.07721300	0.42617100	0.42399900
C	3.10317300	-0.88416300	0.09942200
O	1.89067200	-0.84639000	0.17037900
O	3.75951200	-2.00518000	-0.14351000
H	4.71473200	-1.75029700	-0.18476100
H	-3.02643100	0.77142800	2.20159700
S	-3.58030600	-0.25359800	1.52329000
C	-4.17987300	0.73820600	0.08562400
H	-5.07283300	0.22440300	-0.27448000
H	-4.48510400	1.71368300	0.45770000
C	-3.18557300	0.91046900	-1.07199500
H	-3.64971000	1.63283700	-1.76110400
N	-2.89691600	-0.37506300	-1.72841200
H	-3.76945800	-0.77902000	-2.05989900
H	-2.33074500	-0.21258400	-2.55718300
C	-1.92370000	1.61504400	-0.57187800
O	-1.95498800	2.64424400	0.04987300
O	-0.78221500	0.97238600	-0.89869700
H	-0.01288000	1.48092000	-0.54662100
Rb	-0.75465800	-1.96057600	0.00273700



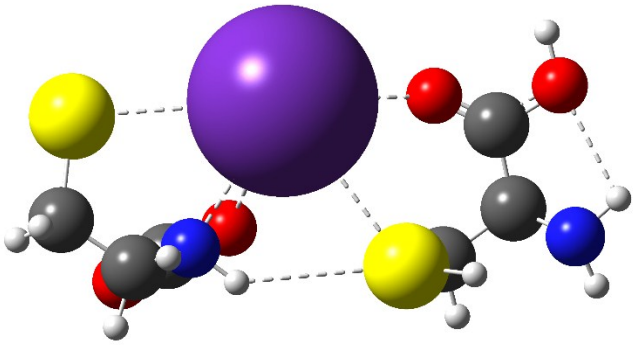
Iso 19 (23.99 kJ/mol)

H	6.01940400	0.55677200	-0.92734800
S	4.72914200	0.70569100	-1.28754400
C	4.11377600	1.39485900	0.30878300
H	4.93501400	1.89090700	0.82420900
H	3.37259100	2.15036600	0.05142500
C	3.47090400	0.34246600	1.22559700
H	3.15761800	0.85215500	2.14508200
N	4.30581100	-0.80297500	1.59878700
H	4.98496200	-1.01664900	0.87221500
H	4.79432700	-0.66633100	2.47571600
C	2.16513200	-0.20161500	0.61911400
O	1.33007900	0.47331100	0.05499300
O	1.99052100	-1.51253900	0.79081900
H	2.82152000	-1.81548100	1.25055100
H	-2.81667600	0.08261000	2.44142100
S	-3.45674800	-0.71393000	1.56222500
C	-4.31818600	0.63669000	0.64271900
H	-5.25685500	0.20464000	0.29205400
H	-4.55938400	1.42252400	1.35487100
C	-3.54927000	1.22633400	-0.54754500
H	-4.13309400	2.09681000	-0.88605800
N	-3.36742400	0.22886500	-1.61514600
H	-4.27844800	-0.12540500	-1.89547400
H	-2.97511800	0.67849500	-2.43829400
C	-2.22034700	1.80981900	-0.06816900
O	-2.10911500	2.50425200	0.90585200
O	-1.17907400	1.45770400	-0.85704600
H	-0.35477100	1.80561900	-0.47340000
Rb	-0.83430900	-1.58377300	-0.80019700



Iso 20 (25.16 kJ/mol)

H	-2.94219300	-1.43527700	-1.94643900
S	-1.76857200	-1.34940300	-1.28527800
C	-2.49043100	-1.55734800	0.39538300
H	-2.70842600	-2.61494700	0.55097900
H	-1.71042700	-1.27027900	1.09971800
C	-3.76980100	-0.74934700	0.63833000
H	-4.06295600	-0.94377800	1.68696800
N	-4.80687800	-1.13047900	-0.31771900
H	-5.15596400	-2.06145800	-0.11446300
H	-5.59401600	-0.49222200	-0.29464100
C	-3.52475800	0.75627000	0.61517200
O	-2.45234100	1.29592400	0.78611400
O	-4.66189000	1.44291500	0.44960200
H	-4.47175700	2.39281900	0.49934800
H	4.27391800	1.16297300	1.35925600
S	3.97525400	1.34293700	0.05710600
C	4.25424300	-0.40049800	-0.48143800
H	4.65992000	-0.33457400	-1.49235500
H	5.02388900	-0.83657600	0.15190500
C	3.00533800	-1.30284400	-0.50833800
H	3.37037800	-2.31920400	-0.72064500
N	2.03284300	-0.82401600	-1.49210100
H	2.46200100	-0.81505300	-2.41324800
H	1.24238300	-1.46230600	-1.54951600
C	2.34963300	-1.37238100	0.86549700
O	1.24108900	-0.96651300	1.13398500
O	3.16269400	-1.94374500	1.76294800
H	2.71119700	-1.97835900	2.62123000
Rb	0.26355700	1.51139000	-0.25209300

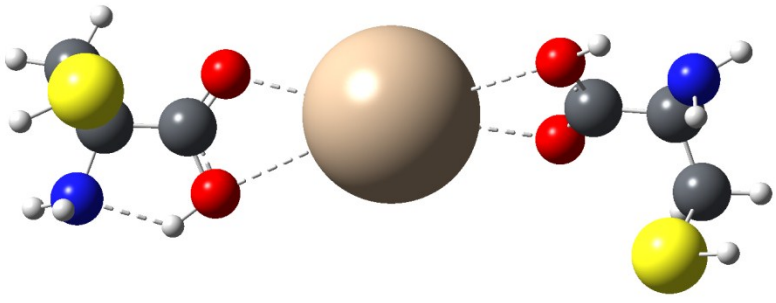


Atomic Coordinates $[(Cys)_2Cs]^+$

Note: Energies include thermal correction at 298 K

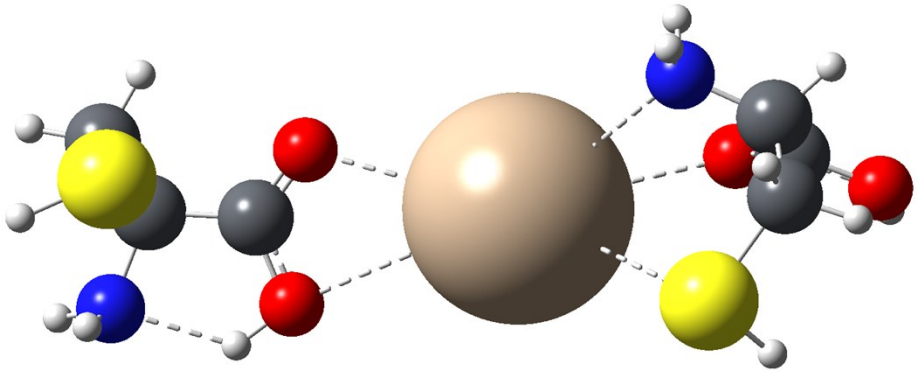
Iso_1 (GM)

H	-6.60548400	0.82445400	2.29691500
S	-5.46045200	1.26393400	1.73779600
C	-5.86376200	0.82640600	-0.00809800
H	-6.94479700	0.84785900	-0.13955900
H	-5.43044000	1.61220200	-0.62547800
C	-5.29848700	-0.53220900	-0.44916000
H	-5.61761600	-0.70019200	-1.48521000
N	-5.69422700	-1.70103500	0.34132300
H	-5.84673600	-1.45201200	1.31565100
H	-6.52714500	-2.15386200	-0.01551000
C	-3.76046900	-0.49554400	-0.51977900
O	-3.11937500	0.44346600	-0.93678800
O	-3.16776800	-1.61932100	-0.11013200
H	-3.91149700	-2.19981600	0.19915500
H	6.59955800	-0.87366600	2.28374700
S	5.45398900	-1.29930900	1.71510600
C	5.86099800	-0.83123100	-0.02198200
H	6.94212900	-0.85371000	-0.15247900
H	5.42598500	-1.60417900	-0.65421000
C	5.30057100	0.53706000	-0.43867300
H	5.62107900	0.72288200	-1.47124000
N	5.69947300	1.68988800	0.37339900
H	5.85070900	1.42253800	1.34305600
H	6.53393500	2.14668100	0.02534400
C	3.76249300	0.50658300	-0.51096000
O	3.11885800	-0.42262000	-0.94571800
O	3.17296500	1.62426700	-0.08081500
H	3.91819400	2.19670500	0.23962500
Cs	0.00024200	0.00791700	-0.63872300



Iso_2 (7.36 kJ/mol)

H	-6.27819000	2.25342400	0.15989900
S	-5.04947700	2.05557500	-0.35774100
C	-5.35084200	0.37361200	-1.05257600
H	-6.40915400	0.27116400	-1.28892200
H	-4.78799000	0.32455400	-1.98378000
C	-4.89689400	-0.76566200	-0.12747100
H	-5.14680400	-1.71132300	-0.62417400
N	-5.47620700	-0.79514400	1.21828800
H	-5.67674000	0.14421100	1.55300600
H	-6.32266200	-1.34918500	1.27029700
C	-3.36250800	-0.79323700	0.00587100
O	-2.59564600	-0.58553800	-0.90766000
O	-2.92656900	-1.10753900	1.22819800
H	-3.74970300	-1.19402400	1.77605900
H	4.20609800	0.60802600	2.36701700
S	3.44578500	1.46143400	1.65260600
C	4.60130600	1.64583500	0.22558400
H	4.50632400	2.68285300	-0.10087400
H	5.61768400	1.50973200	0.58873300
C	4.33660200	0.72245100	-0.97803300
H	5.19392200	0.85716100	-1.65558200
N	3.05301900	1.03378500	-1.61057000
H	3.04856000	2.00699200	-1.90315600
H	2.94077500	0.48017400	-2.45581100
C	4.35809900	-0.74532900	-0.56774800
O	3.42688900	-1.51131700	-0.65972100
O	5.55871000	-1.09631600	-0.08565200
H	5.54157100	-2.03922800	0.14286100
Cs	0.43847400	-0.56377300	0.04631800

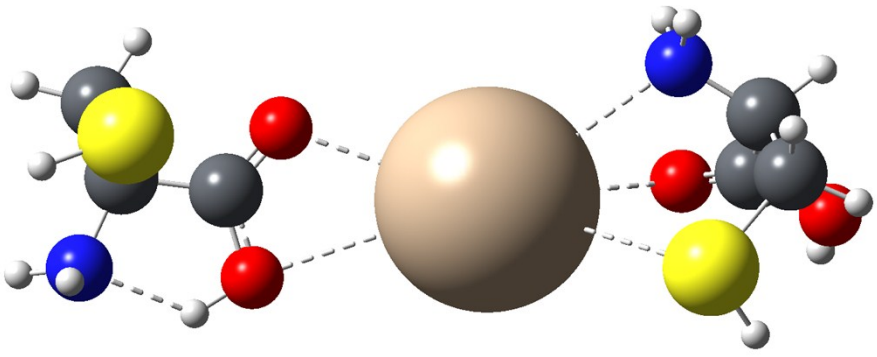


Iso_3 (8.26 kJ/mol)

H	5.70349100	0.74523600	1.83945300
S	4.54963500	0.06935600	1.67316700
C	4.79316500	-0.38694600	-0.09851900
H	5.85884600	-0.37800400	-0.32303400
H	4.43242800	-1.40874300	-0.20733500
C	4.03556900	0.52463900	-1.07495400
H	4.26891700	0.18340900	-2.09121400
N	4.33074100	1.95807100	-1.00190800
H	4.55971900	2.23698000	-0.05058600
H	5.08645000	2.23638200	-1.61650000
C	2.50938600	0.33868800	-0.94827200
O	1.97171900	-0.73177200	-0.76840900
O	1.81740800	1.46673300	-1.09794800
H	2.51025600	2.17291600	-1.19321400
H	-4.98602500	0.00680600	0.67879700
S	-4.39369600	-0.17184800	-0.51875100
C	-3.88744100	1.58359800	-0.78174900
H	-3.98356400	1.76039500	-1.85436600
H	-4.60550900	2.22738000	-0.27819900
C	-2.45059300	1.93795800	-0.35111700
H	-2.36816700	3.03166300	-0.45007800
N	-1.47033700	1.20895600	-1.15248100
H	-1.60069600	1.43710700	-2.13379100
H	-0.51993700	1.48717000	-0.91655000
C	-2.23701300	1.63783800	1.12755700
O	-1.47065000	0.81750700	1.57644500
O	-3.02326300	2.40792700	1.89567600
H	-2.85317200	2.19513800	2.82685800
Cs	-0.81747400	-1.89019900	0.04174600

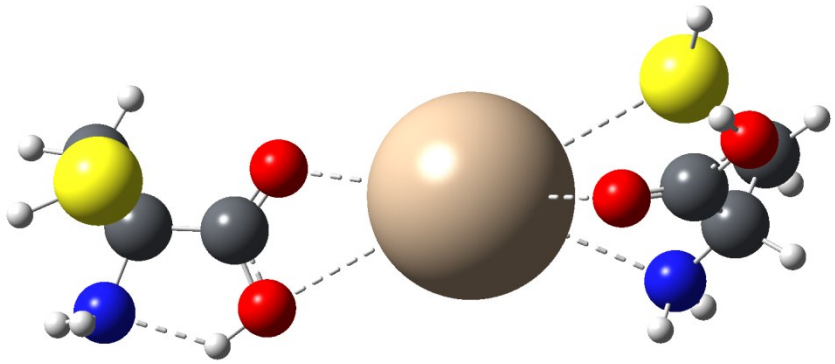
Iso_4 (9.83 kJ/mol)

H	6.35752200	2.16018600	-0.27049200
S	5.11352900	2.03310600	0.23261800
C	5.35617300	0.40283600	1.06089400
H	6.40624600	0.29304100	1.32861200
H	4.77279500	0.43949500	1.97995800
C	4.89208100	-0.79287600	0.21546900
H	5.10687900	-1.70336600	0.78843600
N	5.49837600	-0.93967300	-1.11060300
H	5.73132500	-0.03400700	-1.51077400
H	6.33034900	-1.51749300	-1.10114200
C	3.36059900	-0.79309700	0.04974600
O	2.58062600	-0.49881600	0.92775000
O	2.94215400	-1.18742700	-1.15526200
H	3.77399900	-1.33555500	-1.67615400
H	-4.21955000	0.82167500	-2.30860900
S	-3.49378200	1.61399400	-1.49480500
C	-4.66589000	1.59984900	-0.06934200
H	-4.60866600	2.59651600	0.37154300
H	-5.67420900	1.47185200	-0.45706600
C	-4.37931200	0.55715100	1.02690900
H	-5.24595000	0.58715300	1.70535300
N	-3.11202200	0.83806700	1.70493700
H	-3.14279600	1.77222300	2.10387200
H	-2.98760900	0.19761800	2.48458200
C	-4.34785300	-0.85570300	0.45586000
O	-3.39268900	-1.59711900	0.47493800
O	-5.53133300	-1.18910000	-0.07826800
H	-5.48057300	-2.09973300	-0.40955700
Cs	-0.43318300	-0.47675000	-0.08698900



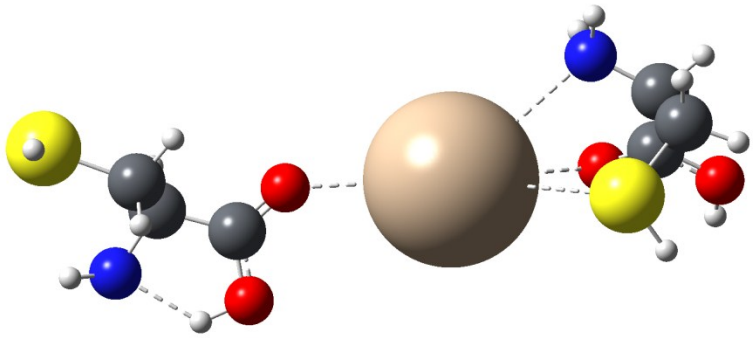
Iso_5 (10.19 kJ/mol)

H	6.55368700	1.98987200	-0.10764400
S	5.28335900	1.90875000	0.33555200
C	5.40332400	0.23426000	1.10004500
H	6.43335600	0.05664200	1.40646800
H	4.78274000	0.26388800	1.99463900
C	4.91533700	-0.89788900	0.18368400
H	5.05472300	-1.84165100	0.72536400
N	5.57396300	-1.02385000	-1.11918100
H	5.86890200	-0.11639900	-1.47154000
H	6.37549200	-1.64284600	-1.09666200
C	3.39497500	-0.80761000	-0.04914500
O	2.59440000	-0.50287500	0.80772000
O	3.01080600	-1.13330100	-1.28294600
H	3.85490400	-1.30701500	-1.77448300
H	-4.28573300	0.09277400	2.41419200
S	-3.88422100	-0.99041900	1.71980800
C	-5.08716400	-0.82176500	0.33061900
H	-5.36372700	-1.84001400	0.05185800
H	-5.98181000	-0.33290400	0.71011900
C	-4.56970800	-0.08971900	-0.92128600
H	-5.44641900	0.05075800	-1.57240600
N	-3.49298000	-0.84380200	-1.56753800
H	-3.83248000	-1.76886300	-1.81612200
H	-3.23018700	-0.39127100	-2.43911500
C	-4.07569300	1.31185600	-0.58283300
O	-2.94550500	1.71199500	-0.74082500
O	-5.06407100	2.06709300	-0.08346000
H	-4.71911000	2.95584700	0.09753200
Cs	-0.43034400	-0.15466600	-0.02129700



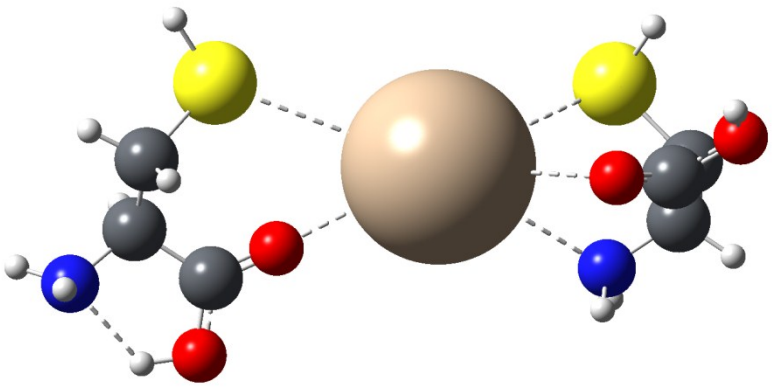
Iso_6 (16.83 kJ/mol)

H	-7.07889400	2.48028000	0.21142100
S	-6.86662600	1.40145200	-0.56701600
C	-5.20569700	0.98106100	0.12018700
H	-4.44946900	1.64046500	-0.30175500
H	-5.22537300	1.10477600	1.20520600
C	-4.85335100	-0.47277900	-0.23225500
H	-4.84868700	-0.57889900	-1.32247300
N	-5.74654700	-1.43845000	0.42191300
H	-6.60552300	-0.99599700	0.73603600
H	-6.01101000	-2.19479500	-0.20020300
C	-3.41114700	-0.74558600	0.23979700
O	-2.43579000	-0.20771900	-0.24510500
O	-3.32118600	-1.61137700	1.23805400
H	-4.25948300	-1.89569600	1.40890200
H	4.49140500	0.19890700	2.39312400
S	3.85837700	1.21061400	1.76670700
C	5.06048200	1.39941100	0.37918900
H	5.10622300	2.46942000	0.16945900
H	6.04252700	1.09410400	0.73382300
C	4.70806200	0.65510000	-0.92186700
H	5.59046900	0.75222600	-1.57311100
N	3.48887700	1.19633200	-1.52708300
H	3.61610900	2.18782700	-1.71037700
H	3.32777600	0.75701300	-2.42963000
C	4.53432200	-0.83947500	-0.67857500
O	3.51682200	-1.46522300	-0.86753100
O	5.66814400	-1.39173700	-0.22494900
H	5.52732600	-2.34423400	-0.10428400
Cs	0.65986000	-0.24057400	-0.06032000



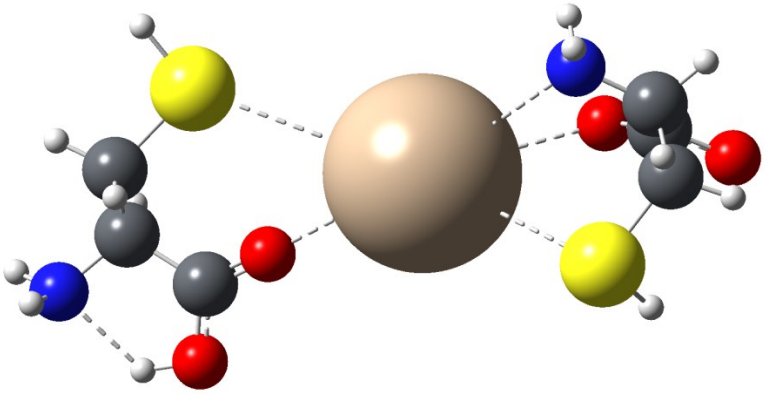
Iso_7 (18.42 kJ/mol)

H	-3.96581200	-3.26057800	-0.33814300
S	-3.35775600	-2.09209600	-0.05209800
C	-4.74888500	-0.99592600	-0.59186600
H	-4.57967800	-0.67715300	-1.62262000
H	-5.65909600	-1.59262900	-0.55780800
C	-4.93951200	0.22368700	0.32420100
H	-4.96814000	-0.12385400	1.36260300
N	-6.17078800	0.98294900	0.07374600
H	-6.43472500	0.98816400	-0.90734400
H	-6.95748200	0.63772900	0.61085300
C	-3.74613900	1.19848900	0.26034800
O	-2.59591900	0.82681600	0.15231500
O	-4.07112500	2.47588200	0.36314000
H	-5.05764600	2.49995100	0.38964300
H	4.33647000	-2.03469800	0.95252900
S	3.68509000	-1.10186800	1.67520300
C	4.75294500	0.32788500	1.20456500
H	4.81838600	0.95529900	2.09509600
H	5.75254600	-0.04637000	0.99448900
C	4.24670900	1.18674000	0.03102100
H	5.06511300	1.88371800	-0.20768100
N	2.99698400	1.86706200	0.37553100
H	3.14351300	2.44870600	1.19578900
H	2.72476500	2.49442200	-0.37657400
C	4.03816400	0.34689400	-1.22360000
O	2.98433700	0.19487800	-1.79664100
O	5.18734300	-0.21208000	-1.62981300
H	5.02003800	-0.71740800	-2.44107500
Cs	0.25607700	-0.22386400	-0.12735300



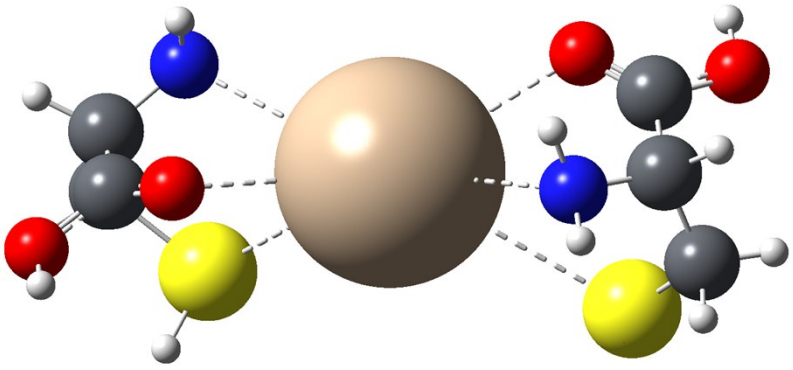
Iso_8 (18.84 kJ/mol)

H	3.93193700	3.22376400	-0.58764300
S	3.34356000	2.07302700	-0.20477300
C	4.72152300	0.95131700	-0.72610000
H	4.50982600	0.55772400	-1.72254600
H	5.62558200	1.55613100	-0.77653700
C	4.96613500	-0.19755200	0.26542100
H	5.03790600	0.22412600	1.27384500
N	6.19260000	-0.96417600	0.01440100
H	6.41081400	-1.04107600	-0.97488700
H	6.99958400	-0.57422300	0.48688400
C	3.78109500	-1.18255700	0.32607000
O	2.62372000	-0.82721000	0.24139100
O	4.12259600	-2.44644600	0.50846400
H	5.10936200	-2.46274900	0.49296800
H	-3.92436800	-2.50697100	-0.43909800
S	-3.47782200	-1.64435700	-1.37351100
C	-4.79540500	-0.37224500	-1.14854100
H	-4.99515600	0.02797300	-2.14401100
H	-5.70026100	-0.87240600	-0.81020800
C	-4.44749700	0.79535900	-0.20714000
H	-5.38124700	1.36357800	-0.07338200
N	-3.35738000	1.60728000	-0.75241800
H	-3.62780700	1.96554800	-1.66410400
H	-3.20114600	2.41813500	-0.15960800
C	-4.06362600	0.29790000	1.18133900
O	-2.99573800	0.47995400	1.71850200
O	-5.07340600	-0.37381500	1.75280300
H	-4.80097900	-0.65258200	2.64143000
Cs	-0.25605700	0.16362500	0.05381800



Iso_9 (20.63 kJ/mol)

H	-3.68497400	2.41781000	-0.67465900
S	-3.19334600	2.05341900	0.52616100
C	-4.51263300	0.83252500	0.94417600
H	-4.67834000	0.92869100	2.01854100
H	-5.42998100	1.13494100	0.44383400
C	-4.18924500	-0.63820700	0.62388100
H	-5.12415300	-1.19602500	0.79002500
N	-3.07878800	-1.12487200	1.44468600
H	-3.31881000	-1.03041700	2.42756100
H	-2.93376200	-2.11701500	1.27785900
C	-3.85165300	-0.82737100	-0.85022700
O	-2.80147600	-1.24575300	-1.27944500
O	-4.88189400	-0.47497300	-1.63287700
H	-4.63974400	-0.63257600	-2.55912700
H	3.68143600	2.41969800	0.67199900
S	3.19622300	2.05112600	-0.53015200
C	4.51766300	0.82873100	-0.93684500
H	4.68938200	0.92138200	-2.01057600
H	5.43224600	1.13266700	-0.43238100
C	4.19231400	-0.64091600	-0.61358500
H	5.12806800	-1.19934800	-0.77275700
N	3.08636000	-1.13012400	-1.43894400
H	3.33170400	-1.03854400	-2.42077700
H	2.94051700	-2.12178500	-1.26998200
C	3.84663900	-0.82525500	0.85927000
O	2.79399700	-1.24184500	1.28417600
O	4.87278900	-0.47074200	1.64633700
H	4.62555300	-0.62520600	2.57177000
Cs	-0.00007300	-0.25077400	-0.00624000

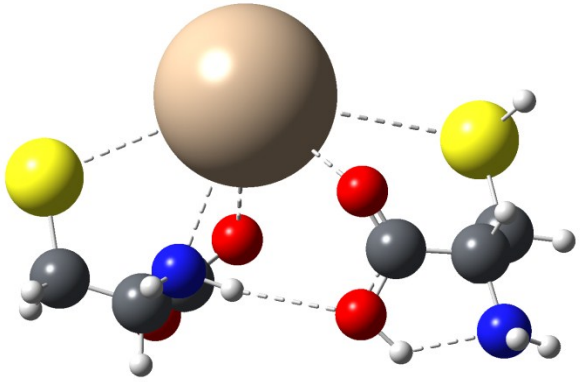


Iso_10 (20.81 kJ/mol)

H	-3.94752600	2.32250100	-0.51520500
S	-3.40279800	1.93182600	0.65420700
C	-4.58152900	0.55333600	0.99630500
H	-4.73101400	0.55288800	2.07733600
H	-5.53590600	0.79695200	0.53449000
C	-4.11788100	-0.84813000	0.56064700
H	-4.98792300	-1.51015900	0.69403900
N	-2.94819200	-1.27878400	1.32781700
H	-3.18028800	-1.29691700	2.31687000
H	-2.69835300	-2.23029300	1.07217300
C	-3.79039700	-0.89210900	-0.92716500
O	-2.71382000	-1.17838500	-1.39776000
O	-4.86170800	-0.57920000	-1.66993500
H	-4.62256200	-0.64565000	-2.60798400
H	3.94378400	-2.32917000	-0.51270000
S	3.40196300	-1.93018500	0.65504700
C	4.58588500	-0.55326400	0.98923100
H	4.74672600	-0.55299500	2.06861100
H	5.53503000	-0.79715800	0.51718300
C	4.11973200	0.84869200	0.55816600
H	4.99106800	1.50961400	0.68820500
N	2.95500500	1.27950400	1.33286900
H	3.18876500	1.27487400	2.32175800
H	2.71815400	2.23931700	1.09661800
C	3.78622500	0.89355000	-0.92802600
O	2.70663400	1.17240600	-1.39582500
O	4.85791100	0.58823900	-1.67412400
H	4.61533100	0.65229200	-2.61142300
Cs	0.00011000	-0.00098800	-0.09284800

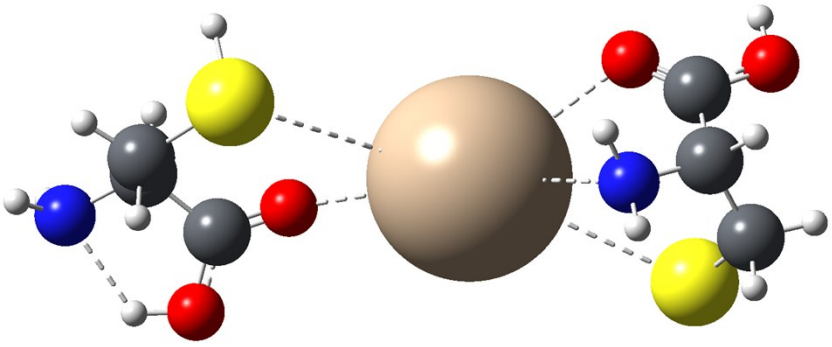
Iso_11 (20.98 kJ/mol)

H	4.29602900	-1.84992500	0.98150900
S	3.35438600	-1.09188500	1.57995600
C	3.96107600	0.53102400	0.98476800
H	3.36064600	1.26894900	1.52208800
H	4.99525800	0.65006700	1.31308000
C	3.90104300	0.80939700	-0.53576000
H	4.46398800	0.03452900	-1.06427300
N	4.40973100	2.16904300	-0.77998800
H	5.07759100	2.46724300	-0.07699800
H	4.86109000	2.25066300	-1.68574300
C	2.45328500	0.74639800	-1.04762800
O	1.87768800	-0.27955600	-1.32129100
O	1.85370600	1.93868000	-1.13267100
H	2.56411500	2.60350900	-0.95741100
H	-4.65248900	-0.14124700	1.05901900
S	-4.21341100	-0.27067000	-0.20868400
C	-3.83035000	1.51246100	-0.49524000
H	-4.09124500	1.70776900	-1.53668300
H	-4.49347900	2.10985200	0.12669100
C	-2.36253200	1.92266000	-0.26987000
H	-2.34237700	3.02184900	-0.34193300
N	-1.48223100	1.26283800	-1.23017300
H	-1.76098100	1.51506700	-2.17390200
H	-0.52039200	1.57712800	-1.11945100
C	-1.91453700	1.59451600	1.14899700
O	-1.02619700	0.83039800	1.44835500
O	-2.63786200	2.27164500	2.05485900
H	-2.31721500	2.04427700	2.94174800
Cs	-0.54500400	-1.85945600	-0.25386500



Iso_12 (22.70 kJ/mol)

H	-3.59479300	2.79348200	-0.59808700
S	-3.34005100	2.17430300	0.57281200
C	-4.83898500	1.11882800	0.59522900
H	-4.88806100	0.71515800	1.60912100
H	-5.70711500	1.76667000	0.46183600
C	-4.92048900	-0.02910000	-0.43821300
H	-4.75938900	0.37974800	-1.44017400
N	-6.21893700	-0.70346800	-0.28774600
H	-6.93964900	-0.09197100	0.07992700
H	-6.55629700	-1.08621200	-1.16519300
C	-3.81156700	-1.06775200	-0.18502100
O	-2.66487900	-0.91784100	-0.54626200
O	-4.20541900	-2.13406900	0.49903100
H	-5.18442700	-2.04651900	0.59146900
H	4.43146500	-2.11181200	-0.77543700
S	3.78126800	-1.97364100	0.39710500
C	4.80155700	-0.58292200	1.05291100
H	4.88204000	-0.75429400	2.12770300
H	5.80194000	-0.66487500	0.63351300
C	4.23932200	0.83127800	0.81871800
H	5.03421200	1.52719500	1.12916800
N	2.98700500	1.03037100	1.55150100
H	3.14900600	0.87720800	2.54296700
H	2.68070200	1.99498000	1.45626600
C	4.00858300	1.10095800	-0.66341000
O	2.94113700	1.35915600	-1.16962200
O	5.15460300	1.02310400	-1.35475900
H	4.97274200	1.22324400	-2.28663000
Cs	0.28304700	-0.23439000	-0.27708700



Iso_13 (22.88 kJ/mol)

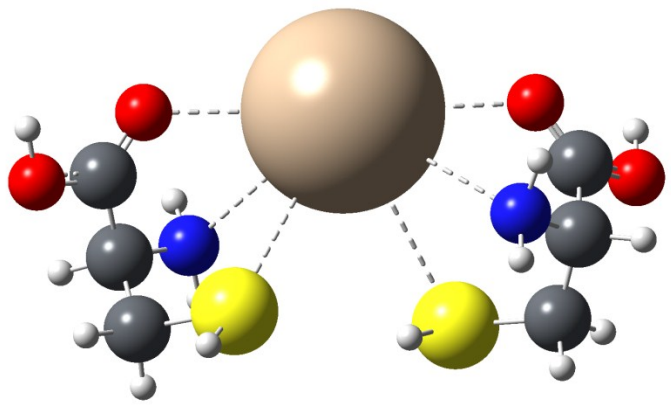
H	-6.19718000	-0.12372400	-0.14594100
S	-5.11918300	0.47847200	-0.68603400
C	-4.02394800	-1.00512600	-0.74003500
H	-4.64105100	-1.90195200	-0.77088800
H	-3.47176200	-0.94574800	-1.67697200
C	-3.03522200	-1.08527200	0.43381800
H	-2.46126600	-2.01419600	0.32422000
N	-3.61347300	-1.05354600	1.77988600
H	-4.47859800	-0.51826100	1.79607300
H	-3.78973900	-1.97784800	2.15499800
C	-1.96724400	0.01759400	0.35319000
O	-1.40812500	0.35975800	-0.67324200
O	-1.64464200	0.55171000	1.52271000
H	-2.26038100	0.11146900	2.17196800
H	1.56772400	-1.78246700	2.08267000
S	2.74837600	-1.21375800	1.77029600
C	3.14590600	-2.33260600	0.35639700
H	4.23369000	-2.41825500	0.34504000
H	2.74085800	-3.31549100	0.58604300
C	2.66163700	-1.87107800	-1.02191300
H	2.88401400	-2.69934200	-1.71625600
N	3.31205800	-0.61526400	-1.42941600
H	4.32102700	-0.73528400	-1.39963400
H	3.07612000	-0.40536800	-2.39512300
C	1.14072100	-1.73371700	-1.05156100
O	0.38266200	-2.40049000	-0.38975000
O	0.73152100	-0.78171800	-1.91016000
H	-0.23308800	-0.65627900	-1.80180200
Cs	1.39509100	1.98283900	0.04124100

Iso_14 (24.56 kJ/mol)

H	3.12006800	3.33593000	0.28575700
S	2.89332200	2.60073500	-0.82209500
C	4.25239300	1.40084100	-0.56658600
H	4.36324700	0.88247300	-1.52174700
H	5.17318600	1.96088500	-0.39380000
C	4.08620400	0.37521700	0.57975700
H	3.84700100	0.90851900	1.50418200
N	5.31640500	-0.42858200	0.67595800
H	6.13223100	0.06348700	0.32807100
H	5.51329100	-0.71584000	1.62936800
C	2.91959400	-0.58739800	0.29378400
O	1.75381000	-0.32429600	0.48702700
O	3.29479800	-1.76040900	-0.21855900
H	4.28326600	-1.75970900	-0.18261400
H	-4.91177100	0.33533000	-0.47064200
S	-3.89328100	0.38481200	-1.35214000
C	-3.22462500	2.02425300	-0.82919800
H	-2.88080000	2.50899600	-1.74435300
H	-4.04301900	2.61927100	-0.42935700
C	-2.05189700	1.97237800	0.16986300
H	-1.86479500	3.01500800	0.47202600
N	-0.89113200	1.32356100	-0.43178400
H	-0.57621400	1.86257600	-1.23283300
H	-0.10309600	1.28504100	0.21091800
C	-2.45566600	1.23898300	1.44232400
O	-1.97554900	0.20315900	1.84086900
O	-3.43516300	1.89121000	2.08792800
H	-3.65754600	1.39875700	2.89368500
Cs	-0.86603300	-2.00649600	-0.15250700

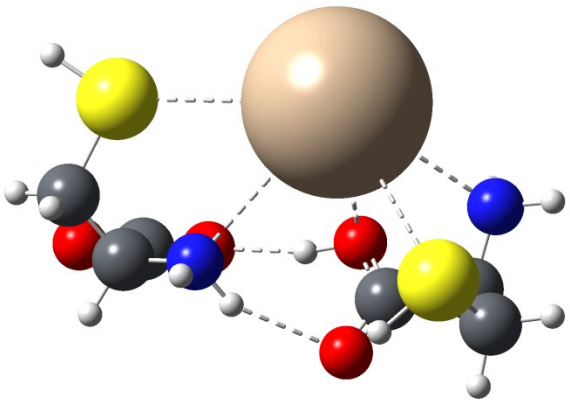
Iso_15 (24.92 kJ/mol)

H	-0.98667400	2.22147400	0.02654400
S	-1.86315200	1.99472800	-0.97303500
C	-3.39242600	1.97987800	0.05150100
H	-3.35063800	2.81322600	0.75416900
H	-4.20732400	2.18017600	-0.64272500
C	-3.68242400	0.67409500	0.81467800
H	-4.66957900	0.81588100	1.28202600
N	-2.62875900	0.36838100	1.78387600
H	-2.52926900	1.14598300	2.43061900
H	-2.89659000	-0.43694200	2.34311300
C	-3.85135500	-0.50177500	-0.14190500
O	-3.17255200	-1.50342900	-0.14800400
O	-4.87464400	-0.30025100	-0.98211400
H	-4.96238600	-1.07323600	-1.56176700
H	2.55148900	2.36786200	2.18639600
S	1.97671800	1.78132200	1.11934600
C	3.41431700	1.96733000	-0.03359300
H	3.27260200	2.86988400	-0.62959000
H	4.32179100	2.07854700	0.55536100
C	3.54571300	0.75738900	-0.96805100
H	4.42766000	0.95127700	-1.59780700
N	2.31581100	0.55990300	-1.73664100
H	2.10400400	1.39988900	-2.26774500
H	2.44126000	-0.18825500	-2.41267100
C	3.86440700	-0.51860300	-0.19132900
O	3.17779900	-1.51415700	-0.17455400
O	5.02847100	-0.41085100	0.46115700
H	5.20608500	-1.24317400	0.92699300
Cs	-0.01837900	-1.43886800	0.09992300



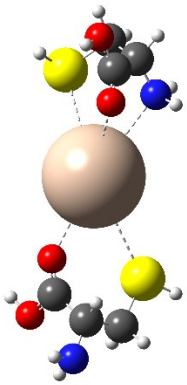
Iso_16 (27.88 kJ/mol)

H	4.43177200	-2.05354800	0.11025800
S	3.21015000	-1.49993900	0.22604600
C	3.71396400	-0.04441200	1.25025800
H	3.68812000	-0.32149800	2.30491700
H	4.73105600	0.23394300	0.98445500
C	2.76581100	1.13731800	1.01124200
H	3.13945300	1.96331300	1.63788400
N	1.38327200	0.76694700	1.31689900
H	1.31903400	0.53758800	2.30515900
H	0.75324300	1.55434700	1.16327600
C	2.86265600	1.66094000	-0.41757200
O	1.92868900	1.83950700	-1.17147100
O	4.11896300	1.95870600	-0.74939100
H	4.13101900	2.31656700	-1.65167400
H	-2.34206600	0.83394700	2.51244900
S	-3.14871100	0.03348700	1.78935400
C	-3.74750900	1.34103300	0.62961100
H	-4.79064500	1.09788800	0.42133000
H	-3.73022700	2.28887500	1.16242600
C	-2.98449200	1.46604700	-0.69168600
H	-3.40663000	2.34836300	-1.20294800
N	-3.10614000	0.24554200	-1.50576600
H	-4.09006300	0.03075600	-1.64374600
H	-2.71650800	0.41309400	-2.42914600
C	-1.51743500	1.82333600	-0.46053900
O	-1.12032600	2.46404500	0.48600000
O	-0.71872900	1.35805600	-1.42983000
H	0.21696600	1.64109800	-1.27618500
Cs	-0.55425900	-1.85049100	-0.36969300



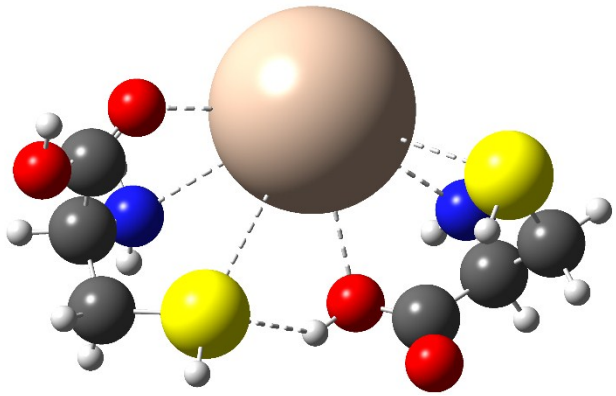
Iso 17 (36.74 kJ/mol)

H	-3.59793400	2.92978700	1.45944500
S	-3.14818800	1.79341900	0.89483800
C	-4.78038400	1.22181300	0.23690900
H	-5.41764500	0.92936700	1.07262600
H	-5.25060800	2.03818700	-0.30726500
C	-4.62467400	0.04737000	-0.74884800
H	-3.98487500	0.37207400	-1.57258900
N	-5.93547900	-0.27018600	-1.28689800
H	-5.88157000	-0.87540500	-2.09802800
H	-6.53890800	-0.70772400	-0.59906700
C	-3.87874000	-1.11335100	-0.07971300
O	-2.67946300	-1.29461700	-0.16025500
O	-4.68730700	-1.90829800	0.63011200
H	-4.16094300	-2.61067600	1.04310800
H	4.19213300	-2.28709000	0.58529900
S	3.65704300	-1.39717200	1.44462000
C	4.80408600	-0.00279800	1.06279800
H	4.96836600	0.51435100	2.00966400
H	5.75821100	-0.42099100	0.74950000
C	4.30105300	1.01597800	0.02360300
H	5.15578700	1.67647300	-0.18930800
N	3.12822300	1.74067400	0.51855200
H	3.36580600	2.21117100	1.38747600
H	2.87040000	2.47036400	-0.14073200
C	3.95954000	0.33959500	-1.29894800
O	2.86559700	0.32376800	-1.81445200
O	5.03882900	-0.24460900	-1.83747100
H	4.78978200	-0.64295100	-2.68655400
Cs	0.22281100	-0.11439800	-0.04517700



Iso 18 (37.22 kJ/mol)

H	1.82308700	3.19945500	1.29272200
S	1.63764900	2.06731100	0.58739600
C	3.32090800	1.99803400	-0.17706800
H	3.37121600	2.69987000	-1.01063900
H	4.05219500	2.28946100	0.57385400
C	3.63819700	0.58318700	-0.68032300
H	4.66608900	0.62706000	-1.07086800
N	2.65848700	0.14522600	-1.67654800
H	2.60269600	0.83025800	-2.42498600
H	2.96345700	-0.72501000	-2.10351700
C	3.67423800	-0.42668900	0.46760000
O	2.95604700	-1.39547400	0.56400200
O	4.62818200	-0.11878000	1.35244100
H	4.63004900	-0.78205200	2.06071800
H	-2.89942900	0.61785200	2.40872600
S	-3.31683100	-0.45604400	1.70943000
C	-4.25020600	0.48187100	0.42270300
H	-5.07800400	-0.16433100	0.12603500
H	-4.67281300	1.36528900	0.89584500
C	-3.44926400	0.88645100	-0.82149300
H	-4.10954300	1.55093100	-1.40310200
N	-3.02534600	-0.28987300	-1.59613800
H	-3.84736800	-0.82886900	-1.85591900
H	-2.59677200	0.01212900	-2.46675300
C	-2.27071600	1.77399500	-0.42668300
O	-2.33981000	2.65035200	0.39376600
O	-1.13873800	1.48534700	-1.11040200
H	-0.42881200	2.08316900	-0.80111000
Cs	-0.14301000	-1.64173800	-0.18851400



Iso 19 (38.58 kJ/mol)

H	4.65416700	-2.52588400	0.52408400
S	3.63453500	-1.72755700	0.15067900
C	4.43706100	-0.12622500	0.61869900
H	4.11848500	0.15919700	1.62351500
H	5.51211800	-0.29862900	0.63123200
C	4.14397600	1.00388100	-0.38133200
H	4.34630800	0.63312800	-1.39205400
N	4.94963000	2.21462700	-0.17991500
H	5.16374800	2.38459000	0.79863800
H	5.82213100	2.19217100	-0.69464400
C	2.65621600	1.40916100	-0.39342100
O	1.74839900	0.61329400	-0.27115600
O	2.43924100	2.70151600	-0.58069000
H	3.33290400	3.12263800	-0.59959100
H	-4.90885900	-0.79562100	0.27674100
S	-4.12745600	-0.82516100	-0.82113000
C	-4.06987900	0.99863800	-1.09791600
H	-3.98429700	1.13247100	-2.17745000
H	-5.02342500	1.41833600	-0.78482400
C	-2.91387400	1.73439900	-0.40269000
H	-3.10472200	2.80957500	-0.55342300
N	-1.61787700	1.31207800	-0.94011400
H	-1.56656500	1.56611400	-1.92290400
H	-0.85298500	1.79920700	-0.47978000
C	-3.02485600	1.55331400	1.10716800
O	-4.03339300	1.75219600	1.72730500
O	-1.86314100	1.16918500	1.70499900
H	-2.02922100	1.18611400	2.66163500
Cs	-0.37483700	-1.59918900	0.06017300