

Table S1. DFT calculated values of bond length and binding energy on each catalytic site.

Cleaved Bond length (Å)				Cleaved Bond length (Å)					
GGE				SSE					
1.42662 Å				1.42469 Å					
Fe(II)				Fe(II)					
	Bonding Site				Bonding Site				
	1	2	3	1	2	3	4	5	
Bond length	1.36741	1.43431	1.47949	1.41161	1.4319	1.47686	1.43525	1.48417	
Gibbs Energy	-239.370211	-200.415707	-301.52	-288.659	-230.465	-313.96	-228.521	-295.47	
Ca(II)				Ca(II)					
	Bonding Site				Bonding Site				
	1	2	3	1	2	3	4	5	
Bond length	1.41911	1.42024	1.46465	1.41119	1.422	1.46217	1.42412	1.4757	
Gibbs Energy	-150.955448	-118.389613	-162.62	-159.175	-131.698	-173.36	-132.642	-171.84	
K(I)				K(I)					
	Bonding Site				Bonding Site				
	1	2	3	1	2	3	4	5	
Bond length	1.41858	1.4247	1.44226	1.41886	1.42456	1.44042	1.42606	1.4473	
Gibbs Energy	-26.1508101	-22.9837721	-34.163	-30.8559	-32.2759	-38.313	-32.6192	-37.333	

GGE – Fe²⁺ - position 1.

C	-2.63842500	0.42204700	0.55914400
C	-1.38905300	0.48331900	-0.06711500
C	-0.72222000	1.68505800	-0.16850600
C	-1.33362900	2.87128900	0.35997600
C	-2.59501000	2.79275600	0.98111600
C	-3.22404900	1.54570600	1.13624700
H	-0.92948000	-0.43087000	-0.42347400
H	-1.12423100	3.85980200	-0.05962500
O	-4.38081700	1.41018600	1.78896800
C	0.77577200	1.73290200	-0.43193500
H	1.13580500	1.20100300	-1.31339000
O	1.18711800	3.12437400	-0.43232300
H	0.88366300	3.61073000	-1.21330900
C	1.47064000	1.24111700	0.86987200
H	0.77521200	1.56338100	1.74837700
C	2.83724000	1.86156400	1.21835100
H	3.38510800	1.20011900	1.89080000
H	3.42383100	2.10744400	0.33358600
O	1.39854600	-0.12438900	0.87170300
O	2.48266200	3.08255600	1.94096800
H	3.23535900	3.66227300	2.11580400
C	1.68367800	-0.78327000	2.08123500
C	2.72503500	-1.69184000	2.10182500
C	0.86904800	-0.56737700	3.19702800
C	2.97801800	-2.40746100	3.26771800
H	3.30713800	-1.84774100	1.20092700
C	1.13653700	-1.27901200	4.36148300
C	2.18556400	-2.19512700	4.38789200
H	3.78455900	-3.12842000	3.29405700
H	0.52738300	-1.13954200	5.24456500
H	2.37558800	-2.74983300	5.29819200
O	-0.14690900	0.34630500	3.05330300
C	-1.18209200	0.31996700	4.04228500
H	-1.58697400	-0.68923200	4.13825300
H	-0.81062800	0.66992000	5.00720100
H	-1.95874700	0.99274200	3.68353200
H	-4.62856800	2.22621700	2.24332100

H	-3.16023800	-0.52492000	0.64952600
O	-3.18314300	3.90963300	1.44535100
C	-4.28676400	4.42075500	0.64696000
H	-4.72992100	5.22053700	1.23316000
H	-3.90062800	4.81090600	-0.29552500
H	-5.02021900	3.63522300	0.45409600
Fe	0.56070400	3.31714200	1.44879800

GGE – Fe²⁺ - position 2.

C	-2.79152800	0.14180800	-0.56332200
C	-1.46052600	0.50160200	-0.37894900
C	-1.11208600	1.78293700	0.05298700
C	-2.10625100	2.73495500	0.28660000
C	-3.42373500	2.37708900	0.08911100
C	-3.75843600	1.09344300	-0.32439700
H	-0.68526800	-0.22544700	-0.58119200
H	-1.81000200	3.73202200	0.58554200
O	-5.13759900	0.87221400	-0.49275200
C	0.33620400	2.19099500	0.24041600
H	0.91145600	1.80406500	-0.61294600
O	0.36474600	3.59252200	0.28411500
H	1.27105300	3.87146300	0.48118700
C	0.93910400	1.61257600	1.54071200
H	0.48661400	2.13325100	2.38585600
C	2.46318900	1.74692500	1.56530600
H	2.84597000	1.41163200	2.53442100
H	2.88220600	1.10852900	0.77736700
O	0.59529300	0.22015200	1.55453600
O	2.76958800	3.10966300	1.34332100
H	3.72049900	3.25122200	1.35481900
C	1.14263800	-0.65689200	2.42552300
C	1.50512600	-1.90506500	1.92456000
C	1.28017300	-0.38898700	3.82418700
C	2.02137700	-2.87423400	2.76411400
H	1.38726800	-2.08158400	0.86255000
C	1.81666000	-1.37524600	4.65883300
C	2.18092000	-2.60201300	4.13453500
H	2.31768700	-3.83625900	2.36603100
H	1.93942200	-1.18622700	5.71619000

H 2.59310000 -3.35909000 4.78986500
O 0.86914000 0.81134100 4.23672300
C 0.97924600 1.14023100 5.62485900
H 0.38192100 0.45208400 6.22620700
H 2.02424800 1.11268100 5.94013700
H 0.59139000 2.15019700 5.71871600
H -5.35216000 -0.00610300 -0.83618800
H -3.05987200 -0.85336800 -0.90079200
O -4.51598400 3.24042200 0.24757100
C -4.25771500 4.63278700 0.58344200
H -5.22761200 5.12775600 0.59141500
H -3.78577000 4.68715800 1.56347000
H -3.62782200 5.06210000 -0.19403100
Fe -6.19680700 2.28308300 0.34923300

GGE – Fe²⁺ - position 3.

C -2.37109600 0.33219700 -1.99075800
C -1.48480900 1.39359900 -1.72239000
C -1.13697200 1.68410300 -0.39171700
C -1.72061500 0.94470500 0.66402300
C -2.68334500 -0.05147400 0.40142500
C -2.95074400 -0.41595000 -0.95589600
H -1.02470400 1.93187000 -2.54206000
H -1.42619400 1.18188700 1.67992900
O -3.75367500 -1.42656400 -1.25190900
C 0.06087300 2.54565700 -0.04384100
H 0.29794600 3.19649200 -0.89274500
O -0.29525900 3.26570400 1.09582100
H 0.40842100 3.90393600 1.28321000
C 1.29563100 1.64814700 0.28964000
H 1.18705100 1.30866200 1.32470100
C 2.58798900 2.44553800 0.09757600
H 3.41687500 1.96771700 0.62247000
H 2.81075300 2.50732700 -0.97521800
O 1.27182400 0.43873700 -0.56220200
O 2.31469300 3.72002700 0.63914400
H 3.11504400 4.25268200 0.68556800
C 2.19446000 -0.59108400 -0.26035300
C 3.56110500 -0.46241600 -0.42398500

C 1.64385900 -1.81186800 0.12601900
C 4.38057500 -1.54480700 -0.11268100
H 3.98668100 0.45008400 -0.81765300
C 2.44854000 -2.89202200 0.43376900
C 3.82999800 -2.74017700 0.32804800
H 5.45199600 -1.45179500 -0.23412400
H 2.02937200 -3.84311400 0.73404900
H 4.47162000 -3.57889400 0.56618300
O 0.24071900 -1.86557100 0.10439900
C -0.41457400 -3.03193700 0.66087100
H -0.19067300 -3.89997200 0.04246300
H -0.07542000 -3.17488500 1.68627300
H -1.48116100 -2.81716900 0.63579500
H -4.21325700 -1.76077900 -0.46674100
H -2.59406200 0.03658600 -3.01104600
O -3.30335300 -0.78823700 1.29563800
C -3.20595200 -0.45355400 2.70201200
H -3.90247400 -1.11904300 3.20175200
H -2.18929700 -0.63583000 3.05338700
H -3.49990300 0.58540600 2.85197300
Fe -0.56106600 -0.29945700 -0.72330200

SSE – Fe²⁺ - position 1.

C -2.88288600 2.78639800 2.24539000
C -1.99970500 1.64757400 2.24304400
C -1.51355200 1.17700100 1.07624400
C -1.87183700 1.80406200 -0.18881900
C -2.66915500 3.01839100 -0.14349600
C -3.10450400 3.54747200 1.06885100
H -1.76075200 1.21719500 3.20938000
H -2.33491700 1.09139600 -0.89224600
O -3.80699400 4.72152200 1.12019300
C -0.39787900 0.16733900 0.98825400
H -0.62364800 -0.77668600 1.49100600
O -0.19161100 -0.10093800 -0.41273300
H 0.48412600 -0.85232100 -0.50762700
C 0.91978000 0.76731000 1.57024800
H 0.89474900 0.69938300 2.66351500
C 1.18528700 2.21610600 1.19151700

H	0.38529500	2.89139000	1.48632300	C	-1.29688200	0.79791700	-0.31631300
H	2.12441100	2.54006800	1.63952700	C	-1.07215600	2.10147200	0.15254600
O	2.01353400	0.05598100	1.03139600	C	-2.11992900	3.00664500	0.33633400
O	1.31426700	2.34813300	-0.25389600	C	-3.39859000	2.57308600	0.04958900
H	2.19208400	2.01731700	-0.50023400	C	-3.62469300	1.28363700	-0.39815500
C	2.26008400	-1.19472700	1.57292100	H	-0.45979000	0.12193200	-0.44069100
C	2.83233800	-1.30143800	2.84469000	H	-1.89522400	4.00926200	0.67369800
C	2.00201600	-2.32718500	0.80598400	O	-4.94156000	0.92736300	-0.68488800
C	3.15537000	-2.56553900	3.33551900	C	0.33841100	2.56521700	0.45253500
C	2.32608500	-3.58832100	1.28971200	H	0.98074800	2.24878700	-0.38186600
C	2.90424000	-3.68424800	2.55129800	O	0.30934200	3.96068700	0.57266300
H	3.60752200	-2.68339700	4.31037700	H	1.20454800	4.25805500	0.78953100
H	2.14196200	-4.48186100	0.71067200	C	0.89179900	1.93405500	1.75540400
H	3.16442400	-4.66314800	2.93389600	H	0.42708600	2.43866600	2.60470800
O	1.41717300	-2.09332000	-0.42408900	C	2.41638600	2.04377300	1.81408100
C	1.26802000	-3.21246500	-1.31361500	H	2.77569800	1.73961900	2.80056800
H	2.24257200	-3.66346300	-1.50077600	H	2.84068400	1.37611000	1.05287000
H	0.57735200	-3.94400800	-0.89249500	O	0.50381300	0.55627100	1.71649900
H	0.86472600	-2.81089600	-2.24019900	O	2.73962400	3.39544000	1.54770300
H	-3.22170300	5.46493700	1.30723300	H	3.68380900	3.54624000	1.64467900
O	-2.90684000	3.51174000	-1.33778800	C	1.08975600	-0.39013300	2.46921100
C	-3.98672700	4.44154800	-1.62790800	C	1.41104500	-1.60479600	1.81250700
H	-4.12496300	4.36452900	-2.70218700	C	1.31043100	-0.25545700	3.86247100
H	-4.88689900	4.14117900	-1.09685300	C	1.98006800	-2.64557200	2.53111200
H	-3.69483000	5.45118900	-1.35163000	C	1.88919700	-1.30300900	4.56737100
Fe	-0.18206900	1.62840700	-1.29753900	C	2.21635700	-2.47858500	3.89577600
O	3.01901500	-0.13129600	3.49172000	H	2.24909100	-3.57606500	2.05245100
C	3.71085900	-0.17330000	4.74211100	H	2.07673200	-1.22115300	5.62833800
H	3.80414000	0.85956200	5.06586500	H	2.66683600	-3.29160700	4.45181500
H	3.14026400	-0.74134800	5.48005300	O	0.92027900	0.91667800	4.39077400
H	4.70342900	-0.60956500	4.61413100	C	1.10292900	1.11395100	5.79325700
O	-3.36228400	3.06478900	3.41876800	H	0.54268100	0.36730900	6.36016900
C	-4.48710100	3.94806100	3.68260200	H	2.16315300	1.06688800	6.05246300
H	-4.82524200	3.65015100	4.67026300	H	0.71588300	2.10661700	6.00503700
H	-4.15276100	4.98239000	3.69139600	H	-4.97972000	-0.00745100	-0.96250500
H	-5.26361300	3.79463300	2.93796400	O	-4.56760400	3.33470800	0.15529700
				C	-4.44307100	4.73483900	0.53512100
SSE – Fe ²⁺ - position 2.				H	-5.44646300	5.15370100	0.48631300
C	-2.58974600	0.37561100	-0.58607500	H	-4.03836000	4.80033000	1.54415100

H -3.79777500 5.22657800 -0.19094900
Fe -6.12657100 2.16838200 0.22541200
O 1.13054400 -1.62899200 0.49296400
C 1.55813800 -2.77314100 -0.24375700
H 1.31108600 -2.56994500 -1.28303000
H 2.63740300 -2.91156700 -0.14843200
H 1.03535500 -3.67109800 0.09578900
O -3.00385900 -0.82815100 -1.02259400
C -2.00103200 -1.81807400 -1.29435500
H -2.54055500 -2.70841700 -1.60341000
H -1.35179500 -1.47312200 -2.10160100
H -1.41944100 -2.01703900 -0.39187900

SSE – Fe²⁺ - position 3.

C -2.65258600 0.38877000 -0.81859300
C -1.31633600 0.79568800 -1.08669500
C -0.74362000 1.89316700 -0.42927000
C -1.47192100 2.58056300 0.56162600
C -2.79642700 2.18179900 0.85637100
C -3.34234900 1.01456400 0.26728800
H -0.76520900 0.23025500 -1.82867000
H -1.00677000 3.42007000 1.06280500
O -4.54382000 0.56523500 0.64480300
C 0.74501600 2.18552500 -0.49328800
H 1.16647300 1.75245800 -1.40812300
O 0.86165300 3.57548900 -0.45591700
H 1.80354200 3.80096400 -0.48704500
C 1.45698200 1.57284600 0.75309900
H 1.26178000 2.23485900 1.60452100
C 2.95758900 1.44825000 0.50682100
H 3.47509900 1.16699800 1.42645300
H 3.14142400 0.69012600 -0.25890900
O 0.83114000 0.27208200 1.06525900
O 3.34615400 2.73865100 0.07256400
H 4.30014800 2.78747800 -0.04037300
C 1.21394500 -0.35521100 2.26877300
C 2.37047400 -1.13755300 2.36594000
C 0.31094300 -0.29916500 3.32781600
C 2.65556300 -1.73364300 3.59963800

C 0.57911000 -0.89323000 4.54484700
C 1.78023700 -1.59070500 4.66465900
H 3.55214500 -2.32539800 3.72118900
H -0.11374700 -0.84712900 5.37303000
H 2.01861900 -2.06349500 5.60923300
O -0.90589900 0.32384400 3.01471700
C -1.85088300 0.56771000 4.08105500
H -2.21281900 -0.38255200 4.47257100
H -1.36610700 1.15641400 4.85926900
H -2.67028800 1.12624000 3.63149700
H -4.97631200 1.20292600 1.23267900
O -3.58062300 2.73820500 1.76532400
C -3.20503300 4.00494000 2.35465300
H -4.05924800 4.30430100 2.95404200
H -2.32649600 3.87325200 2.98877100
H -3.01943000 4.73726800 1.56876900
Fe -1.14510800 0.50234200 1.07069800
O 3.10605300 -1.26025200 1.25728900
C 4.27550400 -2.08872500 1.30417800
H 4.69286700 -2.06022100 0.30171700
H 4.99798600 -1.69148300 2.01987000
H 4.00484900 -3.11425100 1.56107700
O -3.07534900 -0.63847700 -1.49803600
C -4.45435400 -1.10998700 -1.53650200
H -4.45729700 -1.82476200 -2.35311100
H -4.70971500 -1.59069500 -0.59622100
H -5.12130000 -0.27832500 -1.75059900

SSE – Fe²⁺ - position 4.

C -2.67365200 0.26412900 -0.14008300
C -1.36643100 0.63179900 -0.36784200
C -0.95558000 1.88204100 0.10205000
C -1.83437200 2.73604700 0.77570700
C -3.14610300 2.34374000 1.01339600
C -3.54315400 1.09786000 0.54172200
H -0.67597900 -0.03263100 -0.87272200
H -1.46574500 3.70174300 1.09780900
O -4.85684000 0.64722500 0.72113800
C 0.48105000 2.31341100 -0.09298200

H	0.79101700	2.03505000	-1.11090700	H	-3.77376900	-2.12657100	-2.16560500
O	0.53895700	3.69821200	0.10024600	H	-3.96033700	-0.34760300	-2.41740900
H	1.46920900	3.96911200	0.10518700	H	-2.33280600	-1.10857500	-2.41913700
C	1.41403100	1.59886400	0.91169900				
H	1.20332500	1.99642200	1.90671200	SSE – Fe ²⁺ - position 5.			
C	2.88817200	1.77479000	0.55290900	C	-1.16344400	0.38298900	-1.40165600
H	3.49504700	1.28981900	1.32581900	C	-0.29241700	1.36877300	-0.86167000
H	3.07795400	1.28073400	-0.40636700	C	-0.73633700	2.18826600	0.20021700
O	1.16297200	0.18661600	0.86205800	C	-2.05668000	2.15404100	0.57570300
O	3.14670500	3.16448000	0.48645000	C	-2.94288700	1.27925100	-0.09420400
H	4.07033300	3.33102900	0.27802000	C	-2.48665900	0.31605300	-1.04127400
C	1.26610200	-0.52446600	2.00132500	H	0.55110900	1.68904900	-1.48181700
C	2.22455600	-1.57764400	2.04703200	H	-2.40034400	2.79456700	1.37779400
C	0.43295600	-0.27812200	3.11141200	O	-3.28364500	-0.68441800	-1.46148000
C	2.35382900	-2.34233700	3.20663400	C	0.31196500	3.01988700	0.87178100
C	0.58998900	-1.02950500	4.26609400	H	0.83039300	3.58595400	0.08725400
C	1.54841000	-2.05216100	4.29625400	O	-0.29203300	3.88831200	1.78081900
H	3.08128200	-3.13888900	3.26907500	H	0.33794000	4.58408500	2.00821600
H	-0.01737200	-0.84489900	5.14091400	C	1.40855200	2.16995400	1.62484000
H	1.65820500	-2.63480600	5.20274100	H	1.21207200	2.31473500	2.68523700
O	-0.48725500	0.70125900	2.93537500	C	2.78522100	2.70569400	1.26891100
C	-1.21722900	1.12431100	4.07870500	H	3.54635900	2.21903900	1.87886700
H	-1.85682800	0.32026600	4.45471400	H	2.99531500	2.51795200	0.20488800
H	-0.54436500	1.45902600	4.87209900	O	1.41934300	0.70126400	1.41130900
H	-1.83232400	1.95834800	3.74667000	O	2.67419500	4.08825500	1.53480400
H	-5.36773200	1.30276300	1.23215300	H	3.52076300	4.53113200	1.42452600
O	-4.12165700	3.01875700	1.64642400	C	1.16702500	-0.08891900	2.55215500
C	-3.84574300	4.36814600	2.06063900	C	0.23403200	-1.11076900	2.42050900
H	-4.76907100	4.73842300	2.49560100	C	1.87005600	0.06505900	3.75420800
H	-3.04941900	4.37441800	2.80697800	C	-0.08457200	-1.95415500	3.46823000
H	-3.56702200	4.97219400	1.19606700	C	1.54462400	-0.77489300	4.82280600
Fe	-4.73507700	-1.29388700	0.63229900	C	0.57764700	-1.75692100	4.67602600
O	2.95281700	-1.71687400	0.94302600	H	-0.80968000	-2.74852800	3.36461000
C	3.96369400	-2.72632200	0.91757000	H	2.05939700	-0.67108700	5.76764800
H	4.42635600	-2.65292000	-0.06212600	H	0.34498700	-2.40014800	5.51516100
H	4.70720700	-2.54187000	1.69614200	O	2.81024000	1.01996200	3.78443000
H	3.51800400	-3.71509400	1.04638300	C	3.57100300	1.18911500	4.98839800
O	-3.23466600	-0.96346300	-0.55349200	H	2.91844500	1.47182400	5.81621300
C	-3.33792400	-1.14196000	-2.00480900	H	4.11867900	0.27486900	5.22270600

H	4.26980000	1.99442600	4.78047800	O	1.52654000	2.67046600	-0.09322800
H	-4.20176900	-0.50364400	-1.21136200	H	2.34174200	3.18488900	-0.13940900
O	-4.22569400	1.15920700	0.17280800	C	2.23731900	-0.36435800	2.64783200
C	-4.86308100	2.04831300	1.11567500	C	3.57045400	-0.11334000	2.90860800
H	-5.91302000	1.77386000	1.10206000	C	1.44073000	-1.10253300	3.53231800
H	-4.44394100	1.89442500	2.11055000	C	4.14052300	-0.59631300	4.08420300
H	-4.73615400	3.08030500	0.78799400	H	4.15862300	0.43147200	2.17902800
Fe	0.72570100	-0.26644800	-0.20411600	C	2.01462800	-1.57611100	4.70693600
O	-0.29945500	-1.24696500	1.13256000	C	3.35918500	-1.31952500	4.97340800
C	-1.36835700	-2.19836100	0.92667000	H	5.18579100	-0.41298100	4.29483000
H	-1.66181400	-2.10648000	-0.11582700	H	1.43223900	-2.15369100	5.41189500
H	-1.00518700	-3.20464000	1.13334800	H	3.79410100	-1.70116200	5.88853200
H	-2.20296000	-1.93644800	1.57674700	O	0.14587900	-1.28978000	3.15144900
O	-0.39805400	-0.62434000	-1.94817600	C	-0.65311700	-2.14682400	3.96882900
C	-0.92317700	-1.57881900	-2.92512400	H	-0.20148700	-3.13826000	4.03821200
H	-0.05218200	-2.10469900	-3.30473000	H	-0.78142600	-1.72208300	4.96663400
H	-1.62702500	-2.25415800	-2.44586400	H	-1.61930900	-2.21998300	3.47597500
H	-1.40737900	-1.01188600	-3.71776900	H	-4.64530100	4.70356300	-0.73549900

GGE – Ca²⁺ - position 1.

C	-3.13960900	2.06024100	-1.61131600
C	-2.17856700	1.18149900	-1.09887300
C	-1.52588200	1.45251700	0.11571400
C	-1.92330000	2.57682000	0.85901000
C	-2.91906400	3.42522100	0.38015800
C	-3.50922700	3.18824600	-0.88808100
H	-1.99123400	0.24104400	-1.61284000
H	-1.50206100	2.76444800	1.83772300
O	-4.42698200	4.01046000	-1.37607700
C	-0.42898300	0.50428000	0.57470900
H	-0.84218000	-0.40052900	1.02715200
O	0.27177100	0.10006500	-0.64197500
H	0.99784200	-0.48153400	-0.35254300
C	0.63912800	1.03286100	1.55156300
H	0.21282000	1.02819600	2.56015000
C	1.22718100	2.42069300	1.32048700
H	0.56888200	3.22020900	1.65575000
H	2.16196300	2.47016700	1.88142500
O	1.67643100	0.07036100	1.44444100

GGE – Ca²⁺ - position 2.

C	-2.62666600	0.25096800	-0.97116500
C	-1.28736800	0.67451700	-1.00335700
C	-0.85568700	1.71786900	-0.18382000
C	-1.78509300	2.38179700	0.64159400
C	-3.13106900	2.00510400	0.64081200
C	-3.55475300	0.90287500	-0.15694900
H	-0.59006800	0.18639100	-1.67603200
H	-1.44490200	3.23374700	1.22028400
O	-4.82289000	0.50089300	-0.14618700
C	0.60213800	2.11955200	-0.11111500
H	1.09380400	1.82496800	-1.04655700
O	0.63616100	3.50450900	0.08082700

H	1.55986200	3.79239200	0.05352600	C	-3.59170000	1.07933800	0.65774000
C	1.33147900	1.43668200	1.07849700	H	-0.76979700	-0.41443400	-0.42660800
H	1.10930600	2.01932700	1.97992200	H	-1.38003200	3.67846300	0.65015400
C	2.83580700	1.36972300	0.83018100	O	-4.97935800	0.87587700	0.86157300
H	3.36330100	1.05482400	1.73506200	C	0.51332500	2.00076000	-0.18613500
H	3.02880300	0.64638500	0.02749400	H	0.77660200	1.54293500	-1.15132800
O	0.79296300	0.08883700	1.27473000	O	0.61346100	3.39900400	-0.23897300
O	3.20246800	2.67702100	0.44619900	H	1.55199400	3.64025200	-0.17641500
H	4.15556700	2.75049700	0.33661800	C	1.44066700	1.40007800	0.89055600
C	1.25201100	-0.58479500	2.41682900	H	1.21638800	1.88407200	1.84695100
C	2.33894200	-1.44506200	2.36070000	C	2.91537400	1.57811100	0.54021600
C	0.53935200	-0.41622000	3.60992700	H	3.51807300	1.13126400	1.33650300
C	2.73995500	-2.10568600	3.51551100	H	3.12361800	1.05612600	-0.40064000
H	2.85994100	-1.58116400	1.42010100	O	1.15613500	0.00959400	0.94239300
C	0.93672600	-1.07814700	4.76312300	O	3.16625200	2.97126400	0.42395100
C	2.04880300	-1.91241300	4.70888000	H	4.10305700	3.13810500	0.28851400
H	3.59226000	-2.77231600	3.48402400	C	1.43099000	-0.60803900	2.14829200
H	0.39477300	-0.95085000	5.69182700	C	2.48246700	-1.50170000	2.24193700
H	2.36681900	-2.42645900	5.60725900	C	0.60201200	-0.36175300	3.25157700
O	-0.60440700	0.38678000	3.53459500	C	2.73813100	-2.15359100	3.44606100
C	-0.94412800	1.15523700	4.71714500	H	3.08829300	-1.68141100	1.36129400
H	-1.36683200	0.50314700	5.47997500	C	0.86737000	-1.00257100	4.45636900
H	-0.04853200	1.65526800	5.08453100	C	1.93551600	-1.89512600	4.54640200
H	-1.68395400	1.88760200	4.40216300	H	3.56080200	-2.85281700	3.51900200
H	-5.38203300	1.13649400	0.32608200	H	0.25286900	-0.82463300	5.32858900
H	-2.98613400	-0.53852700	-1.62299100	H	2.13011900	-2.38957900	5.48970800
O	-4.11666700	2.58613700	1.32803800	O	-0.43318500	0.51185300	3.04104400
C	-3.89171600	3.88410600	1.90693500	C	-1.22070300	0.84434800	4.16748000
H	-4.85911100	4.21025100	2.27599800	H	-1.73621200	-0.03389000	4.56688000
H	-3.18385900	3.81325200	2.73507900	H	-0.61658900	1.30090200	4.95622700
H	-3.52563400	4.57279700	1.14411700	H	-1.95713000	1.56711700	3.81549800
Ca	-1.48232900	-0.24373100	1.49098000	H	-5.17394900	0.11128300	1.42164000

GGE – Ca²⁺ - position 3.

C	-2.75888900	0.07036500	0.18710700	H	-3.15052900	-0.93026100	0.04000000
C	-1.43165600	0.36542700	-0.07335400	O	-4.03986000	3.36895500	1.19823500
C	-0.93155200	1.66363000	0.10832900	C	-3.61517400	4.34405200	2.20054300
C	-1.77843700	2.67604100	0.54476100	H	-4.51202900	4.87616700	2.50716200
C	-3.10436900	2.38063300	0.83208400	H	-3.18210200	3.80348900	3.03980200
				H	-2.89522300	5.02904300	1.75817300
				Ca	-5.48334800	2.69124000	-0.34023200

SSE – Ca²⁺ - position 1.

C	-3.44663400	2.02170200	-0.76160000
C	-2.50304000	1.01729000	-0.54074000
C	-1.46017700	1.22689800	0.38816900
C	-1.40532500	2.42296900	1.09328000
C	-2.33249900	3.46241800	0.86185400
C	-3.32567300	3.28232300	-0.11712600
H	-2.56787600	0.07566700	-1.07300500
H	-0.63465200	2.62460800	1.82618800
O	-4.17100800	4.27312500	-0.40975700
C	-0.27940300	0.27400800	0.29958200
H	-0.57767300	-0.75640900	0.50216500
O	0.12149700	0.38299800	-1.11299100
H	0.75843100	-0.31436800	-1.32570800
C	0.94610700	0.56527200	1.16932300
H	0.62208900	0.80945300	2.18518500
C	1.93449800	1.60140000	0.59842200
H	2.61758500	1.91647800	1.38594900
H	2.52092100	1.11646900	-0.17998100
O	1.70336100	-0.62553100	1.16463200
O	1.29964900	2.78520000	0.00833900
H	1.71619800	3.57657200	0.36816800
C	2.09099400	-1.11059500	2.40214100
C	3.41688800	-0.95778400	2.80829400
C	1.15386600	-1.77444900	3.19285900
C	3.81952400	-1.52748600	4.01648500
C	1.55536800	-2.33440800	4.40287100
C	2.88593700	-2.20830300	4.78805600
H	4.84139000	-1.44458400	4.35808900
H	0.85905300	-2.86573500	5.03567400
H	3.20334800	-2.65027600	5.72422200
O	-0.11260000	-1.79785600	2.69033900
C	-1.07588800	-2.56088000	3.41371800
H	-0.75961000	-3.60282200	3.49364900
H	-1.23597000	-2.14149600	4.40943300
H	-1.99889500	-2.50444500	2.84162400
H	-4.88311500	3.94907600	-0.98226500
O	-2.13902700	4.59183300	1.54040100

C	-3.26601200	5.38972600	1.98704400
H	-2.88318200	5.96106300	2.82736400
H	-3.60235300	6.05036200	1.19274000
H	-4.07574200	4.73746600	2.31345400
Ca	-0.46029100	2.61196800	-1.44949100
O	4.20764000	-0.23916300	1.97565800
C	5.60098600	-0.19895000	2.27692800
H	6.06777900	0.35225400	1.46482600
H	5.78094600	0.31745100	3.22263200
H	6.01437900	-1.20877000	2.31795400
O	-4.49204100	1.95474600	-1.58852800
C	-4.83642300	0.69533600	-2.18696500
H	-4.98062700	-0.05899500	-1.41195800
H	-5.76772200	0.86853100	-2.71714600
H	-4.06232000	0.38632900	-2.89252100

SSE – Ca²⁺ - position 2.

C	-3.00348900	0.58979600	0.28105500
C	-1.66657300	0.75658800	-0.03435000
C	-1.09088400	2.03272500	0.00008500
C	-1.86164700	3.15727400	0.29295900
C	-3.20452700	2.99082900	0.59097800
C	-3.77729300	1.71866100	0.57920600
H	-1.04353400	-0.09767400	-0.25687000
H	-1.38861100	4.13102100	0.28681200
O	-5.14456900	1.55505200	0.86579400
C	0.39092400	2.22191000	-0.27394200
H	0.62655000	1.72711300	-1.22779400
O	0.62777300	3.60147700	-0.34713900
H	1.55566400	3.77939700	-0.12031900
C	1.24304000	1.52831000	0.81212300
H	0.94371300	1.89681000	1.80071400
C	2.74092500	1.74475600	0.60519600
H	3.28120900	1.16517400	1.35775600
H	3.02503400	1.37817800	-0.38693800
O	0.96471100	0.13951500	0.68617700
O	3.00118400	3.13650900	0.74603900
H	3.94606400	3.30705800	0.70409100
C	1.24847200	-0.64045500	1.78529900

C	2.40008400	-1.43622100	1.79307100	H	-1.37016300	3.34955400	1.31150000
C	0.34450400	-0.69195700	2.84869300	O	-4.81778600	0.64000000	0.04615400
C	2.64453500	-2.27402000	2.88397600	C	0.62769300	2.20865200	-0.08742700
C	0.59360500	-1.51859900	3.94136200	H	1.08456000	1.92542500	-1.04359300
C	1.74470100	-2.29902000	3.94008200	O	0.70124000	3.58837700	0.13395200
H	3.52654300	-2.89757900	2.91570800	H	1.63409900	3.84645500	0.11987000
H	-0.08549400	-1.56432800	4.78088000	C	1.37565200	1.48009500	1.06282800
H	1.94354600	-2.94490500	4.78608700	H	1.20293700	2.05331600	1.98119200
O	-0.76296000	0.10134500	2.71019500	C	2.86706300	1.38207500	0.76406200
C	-1.65064200	0.16436500	3.81176900	H	3.40464700	0.96950200	1.62344700
H	-2.10116300	-0.81145000	4.01651700	H	3.01825700	0.72702300	-0.09961600
H	-1.14391400	0.52598700	4.71017600	O	0.80237600	0.14905400	1.25679900
H	-2.42931400	0.87271800	3.52809300	O	3.26273300	2.71262100	0.49486800
H	-5.29876000	0.61791100	1.08871300	H	4.20759400	2.76155600	0.32215200
O	-4.08500800	4.06340500	0.83792100	C	1.24607300	-0.54851300	2.38306300
C	-3.59544500	5.12041300	1.72035700	C	2.29564400	-1.47813300	2.28296200
H	-4.45558500	5.74006100	1.96045700	C	0.58364100	-0.35594900	3.59917200
H	-3.19092200	4.65469100	2.61700500	C	2.68259900	-2.16393900	3.43649400
H	-2.83746300	5.70128000	1.19980300	C	0.96654400	-1.03812500	4.74319000
Ca	-5.63612100	3.24626400	-0.51237000	C	2.02939000	-1.92964800	4.64086600
O	3.20134500	-1.31536700	0.71488600	H	3.49314000	-2.87862200	3.40033200
C	4.35634000	-2.14464500	0.65226000	H	0.45829100	-0.88887400	5.68620200
H	4.83615300	-1.91425600	-0.29511700	H	2.34839400	-2.46951400	5.52376300
H	5.04127900	-1.92360700	1.47464300	O	-0.51769700	0.50363800	3.54685400
H	4.07707200	-3.20061200	0.67369900	C	-0.78242400	1.30037500	4.72785400
O	-3.68221000	-0.56588700	0.39021400	H	-1.21174300	0.67866700	5.51210700
C	-2.91767200	-1.78808700	0.35107200	H	0.14704500	1.76041100	5.06170000
H	-3.61838300	-2.58056700	0.59522500	H	-1.49518200	2.06388700	4.42487300
H	-2.51445800	-1.94117500	-0.65054700	H	-5.34283600	1.28728600	0.54094800
H	-2.11423300	-1.73972700	1.08894300	O	-4.04517000	2.71072800	1.47834200
				C	-3.78995400	3.98889300	2.08545300
				H	-4.74142600	4.31149500	2.49681000
				H	-3.05481600	3.89004800	2.88641400
				H	-3.44400600	4.69737200	1.33162600
SSE – Ca ²⁺ - position 3.				Ca	-1.46331100	-0.12577000	1.53044400
C	-2.65384900	0.41033200	-0.92479500	O	2.84497400	-1.60823300	1.07290000
C	-1.30268800	0.81698000	-0.95017500	C	3.92067600	-2.54328200	0.91456400
C	-0.84179400	1.84309400	-0.12803200	H	4.20048100	-2.49156200	-0.13333800
C	-1.73213300	2.50864500	0.73204700	H	4.76859100	-2.25945400	1.54081700
C	-3.08274100	2.14090700	0.74408700				
C	-3.54303700	1.04968100	-0.03671500				
H	-0.64288800	0.31163300	-1.64772000				

H 3.58626000 -3.55325600 1.15810000
O -2.99304100 -0.63541500 -1.68162300
C -4.25389900 -0.63171600 -2.40305000
H -4.09003100 -1.28955400 -3.25137800
H -5.05289000 -1.00775000 -1.77005000
H -4.47883500 0.37754500 -2.74773700

SSE – Ca²⁺ - position 4.

C -2.75137400 0.50353900 -0.09164800
C -1.47264000 0.86228700 -0.47492700
C -0.98315800 2.10215700 -0.07186900
C -1.80306700 3.01786200 0.59586300
C -3.11817500 2.68975500 0.89737000
C -3.57795300 1.41072200 0.57322400
H -0.83566700 0.15256600 -0.98588000
H -1.38064800 3.97733100 0.86686900
O -4.90376200 1.04902300 0.86522400
C 0.48274400 2.42280800 -0.25921500
H 0.78663000 2.11957400 -1.27195400
O 0.64878400 3.79714200 -0.05898500
H 1.59106400 3.97501700 0.08786000
C 1.30512500 1.58901600 0.75505700
H 1.03104900 1.91322100 1.76557600
C 2.80905900 1.72848200 0.53854700
H 3.32888500 1.12936700 1.29170600
H 3.06202200 1.33753000 -0.45273100
O 0.94852500 0.22544900 0.55102500
O 3.13230500 3.10602100 0.65782500
H 4.08190000 3.23866600 0.59459200
C 1.08130100 -0.61202200 1.63260300
C 2.15388800 -1.51354000 1.67397700
C 0.12134700 -0.60829900 2.64812000
C 2.25597800 -2.40846300 2.74139200
C 0.23065700 -1.49432500 3.71819300
C 1.29953900 -2.38328000 3.74708700
H 3.07598500 -3.11013900 2.79824700
H -0.49029200 -1.49375500 4.52387100
H 1.39071000 -3.07116600 4.57834600
O -0.89920300 0.29735600 2.50115600

C -1.66186200 0.58765100 3.66289800
H -2.29922000 -0.25620900 3.94561800
H -1.01472100 0.84615600 4.50442800
H -2.28431100 1.44577500 3.40998800
H -5.26671300 1.69266400 1.50097200
O -4.03719700 3.44315100 1.52882500
C -3.63646900 4.74566200 1.99261900
H -4.51324200 5.16938200 2.47239600
H -2.82189000 4.65018400 2.71212100
H -3.33293400 5.36454600 1.14736500
Ca -5.10663100 0.12440800 -1.18354400
O 3.02563800 -1.42665000 0.64999300
C 4.13573300 -2.31818600 0.64718900
H 4.70079400 -2.08535900 -0.25120600
H 4.76370200 -2.16167300 1.52763400
H 3.79951900 -3.35703200 0.60897200
O -3.27843100 -0.77785300 -0.34252100
C -2.58612000 -1.85373000 0.37968800
H -2.64795100 -1.63922200 1.44572500
H -3.09784200 -2.77646500 0.11930200
H -1.54768300 -1.87666800 0.05477700

SSE – Ca²⁺ - position 5.

C -2.20800300 0.24042900 -0.93170400
C -0.96143400 0.87522300 -0.81932800
C -0.85506900 2.07291000 -0.12868500
C -2.01250600 2.73719300 0.28313600
C -3.26077600 2.16470600 0.05226700
C -3.36824200 0.85976700 -0.49321900
H -0.08673500 0.40070500 -1.26448500
H -1.91688700 3.69593000 0.77649200
O -4.54397900 0.21858100 -0.55065200
C 0.51096200 2.55942400 0.27616500
H 1.23179900 2.30480000 -0.51264700
O 0.43947600 3.93877100 0.48238700
H 1.32942100 4.26630800 0.66918400
C 0.97674100 1.89461200 1.61031000
H 0.50925000 2.43923800 2.42942100
C 2.50155000 1.91838800 1.71530200

H	2.82245800	1.67778400	2.73252500	C	-1.46389400	0.34168200	-0.71183100
H	2.91317400	1.17014500	1.02267000	C	-0.84619300	1.45682600	-0.16789700
O	0.51374300	0.49620000	1.69840100	C	-1.58259100	2.33993300	0.63583300
O	2.89709700	3.22165200	1.34985800	C	-2.92029500	2.08903800	0.88108000
H	3.83767800	3.35129500	1.50174000	C	-3.54290900	0.95291300	0.32872600
C	1.15038400	-0.37288000	2.58400900	H	-0.89138600	-0.34951100	-1.31926700
C	1.62167100	-1.59207100	2.08133400	H	-1.09335400	3.19583200	1.08664100
C	1.25997900	-0.09342000	3.96016900	O	-4.84398100	0.70495500	0.57710600
C	2.24646500	-2.51881700	2.90552800	C	0.62351700	1.69506400	-0.37815400
C	1.90592700	-1.01582800	4.78205400	H	0.99167500	1.02120400	-1.15962200
C	2.39623500	-2.20380700	4.24957600	O	0.87289300	3.06159500	-0.79041400
H	2.61166900	-3.45857300	2.51368300	H	0.08868800	3.31783300	-1.29020400
H	2.02300000	-0.81604400	5.83822900	C	1.44288800	1.40890900	0.88193300
H	2.89184400	-2.90899800	4.90499200	H	1.00053700	1.93183500	1.73810100
O	0.74242800	1.07660300	4.35423600	C	2.92425500	1.77337200	0.76109800
C	0.86547600	1.44279500	5.73600500	H	3.50225300	1.12158500	1.41979000
H	0.34625700	0.72060400	6.36834300	H	3.27780400	1.60814400	-0.26095000
H	1.91740300	1.51366400	6.01863800	O	1.34310100	0.00266700	1.03967600
H	0.39326300	2.41663500	5.82312600	O	3.18944200	3.14591900	1.08151800
H	-5.25170800	0.81715700	-0.26655000	H	3.27037700	3.22993400	2.03569500
O	-4.44415100	2.68588900	0.38218100	C	1.53578600	-0.47589200	2.31811200
C	-4.49234400	4.01501700	0.92032100	C	2.63948100	-1.26607300	2.59003000
H	-5.54649900	4.24316900	1.04278800	C	0.57302000	-0.23032000	3.31249700
H	-3.98797200	4.04724100	1.88766700	C	2.81686200	-1.81541500	3.85843600
H	-4.03486200	4.71685900	0.22133800	H	3.33851900	-1.46608500	1.78591800
O	1.33830000	-1.83870200	0.73739500	C	0.75826700	-0.77518200	4.57983900
C	2.29984700	-2.62755600	-0.01013500	C	1.87801700	-1.56265200	4.84630400
H	2.05316200	-2.49232500	-1.06022100	H	3.67645400	-2.44029600	4.06307300
H	3.30094500	-2.25075400	0.19519600	H	0.02807100	-0.60589400	5.35973400
H	2.21680900	-3.67843000	0.26332800	H	2.00149300	-1.98557900	5.83551700
O	-2.15863900	-1.12521100	-1.20250700	O	-0.48572000	0.53366200	2.94210400
C	-2.91382300	-1.61786000	-2.35032700	C	-1.58195100	0.61270400	3.83844500
H	-2.71289600	-2.68398800	-2.40722600	H	-1.95122400	-0.38548900	4.08728900
H	-3.97217300	-1.42871400	-2.18877000	H	-1.30667900	1.14305500	4.75499500
H	-2.55030900	-1.11024700	-3.24266900	H	-2.35950300	1.16410200	3.31335700
Ca	-0.85848600	-1.12157200	0.77122200	H	-5.19976000	1.41440300	1.12627000
				H	-3.30909200	-0.78045500	-0.87747000
GGE – K ⁺ - position 1.				O	-3.74434400	2.84114700	1.66523700
C	-2.81095400	0.08718000	-0.46375800	C	-3.21486800	4.01901300	2.24296800

H -4.02508100 4.47277800 2.80784300
H -2.38531100 3.78291300 2.91716200
H -2.87577300 4.71174700 1.46719400
K 2.85392400 4.72484100 -0.86954000

GGE – K⁺ - position 2.

C -2.69553800 0.30725700 -1.10117300
C -1.34370600 0.65458500 -1.01571900
C -0.93020100 1.68800400 -0.18371200
C -1.88201000 2.40308600 0.55705000
C -3.22776800 2.07078600 0.46529700
C -3.64041400 1.00562000 -0.36285000
H -0.61616900 0.12246100 -1.61817600
H -1.55128000 3.24431100 1.15345400
O -4.94415200 0.67194200 -0.44439400
C 0.52703300 2.07100500 -0.06979600
H 1.04825700 1.72070500 -0.97120900
O 0.58601200 3.47339200 0.03894100
H 1.51425000 3.72506500 0.13113000
C 1.21309500 1.44038800 1.16339500
H 0.89664500 2.00374900 2.04785400
C 2.73462900 1.46306100 1.02572400
H 3.20416200 1.10933900 1.94830200
H 3.01731600 0.79338300 0.20355300
O 0.77297600 0.07238400 1.28571600
O 3.11110200 2.80072300 0.74810400
H 4.06609700 2.86979400 0.67394300
C 1.26697700 -0.60952900 2.38462700
C 2.24638000 -1.57721500 2.22140100
C 0.73236600 -0.35359600 3.65685000
C 2.72814000 -2.27531700 3.32433700
H 2.62689800 -1.76160400 1.22339900
C 1.22486400 -1.04236700 4.76060300
C 2.22510900 -1.99625600 4.58819800
H 3.49682700 -3.02610400 3.19502500
H 0.83455000 -0.84682200 5.75066400
H 2.60242400 -2.52727300 5.45298800
O -0.29600800 0.55525000 3.70640300
C -0.60659400 1.12152800 4.97987600

H -1.06718700 0.38144000 5.63810700
H 0.29508900 1.52360300 5.44594500
H -1.31071200 1.92792600 4.78823500
H -5.46823500 1.33675800 0.02165500
H -3.03893900 -0.47443700 -1.76851300
O -4.24720200 2.69498500 1.10673800
C -3.96559100 3.92652000 1.76216500
H -4.92172900 4.30682400 2.11075800
H -3.30107400 3.76754000 2.61566600
H -3.51253900 4.63531000 1.06552000
K -1.79674700 -0.52361900 1.72531800

GGE – K⁺ - position 3.

C -2.67545100 0.00429300 0.09748500
C -1.36696700 0.35026100 -0.21650200
C -0.89723100 1.62706400 0.06279500
C -1.75007500 2.56463100 0.64206200
C -3.05793300 2.22283600 0.95218600
C -3.51567000 0.93377000 0.68431200
H -0.70846500 -0.38321500 -0.66326800
H -1.36061400 3.55593800 0.82804000
O -4.83626900 0.63709900 1.00425800
C 0.54083200 2.00744000 -0.21216900
H 0.84675400 1.54874100 -1.16358800
O 0.61761300 3.41277300 -0.28263200
H 1.54414000 3.67498000 -0.19333100
C 1.46932400 1.46307300 0.89005500
H 1.19845100 1.94122500 1.83671600
C 2.94753600 1.68956400 0.58711000
H 3.53987300 1.22399600 1.38142000
H 3.18987900 1.20652100 -0.36661500
O 1.26960800 0.05381400 0.95235900
O 3.18750900 3.09041700 0.52850600
H 4.11877700 3.25887600 0.36644400
C 1.47979300 -0.53323600 2.17700800
C 2.53527400 -1.41239300 2.34384800
C 0.58264500 -0.29673400 3.23315900
C 2.72805000 -2.06061000 3.56266300
H 3.19297100 -1.58663500 1.50014500

C 0.78423700 -0.93553400 4.45221800
C 1.85611200 -1.81440400 4.61102800
H 3.55447100 -2.74869600 3.68525000
H 0.11060800 -0.76418000 5.28107900
H 1.99738100 -2.30728600 5.56484600
O -0.43986100 0.55959600 2.96315900
C -1.37974100 0.79738800 3.98893100
H -1.87743400 -0.12982400 4.28999100
H -0.90849700 1.25779000 4.86279500
H -2.11292600 1.48220200 3.56487600
H -4.96176900 -0.31363500 0.91738900
H -3.04589800 -0.99338500 -0.11747800
O -3.97245200 3.09586100 1.51836900
C -3.45748000 4.35573500 1.94967800
H -4.27912600 4.87546000 2.44111900
H -2.64278700 4.21242700 2.66216800
H -3.10746300 4.94472400 1.10004100
K -6.49603600 2.57125800 1.35113300

SSE – K⁺ - position 1.

C -2.86729400 1.13353500 0.51052500
C -1.53266000 1.03682000 0.15345000
C -0.77770200 2.20307100 0.01323300
C -1.39535700 3.43815700 0.16735900
C -2.74573200 3.53958800 0.52305200
C -3.48485500 2.37848400 0.72517400
H -1.05832300 0.07374100 0.03780300
H -0.88562000 4.36856900 -0.05456200
O -4.77243700 2.43811000 1.13847100
C 0.72106300 2.09589600 -0.20772800
H 0.94773300 1.48504500 -1.08732300
O 1.31799700 3.38699600 -0.34904300
H 1.22607600 3.67665400 -1.26104700
C 1.40340100 1.38786600 0.98572300
H 0.87849700 1.63252600 1.92074400
C 2.87836100 1.73591900 1.15930400
H 3.36457700 0.91443500 1.68879600
H 3.36357400 1.88141300 0.19143700
O 1.23982400 0.00386400 0.71934900

O 2.95229600 2.93470400 1.94665700
H 3.86606000 3.07320300 2.20935800
C 1.46598400 -0.84709300 1.77831500
C 2.61450600 -1.64570500 1.77737800
C 0.51703400 -0.97492100 2.79849500
C 2.80666700 -2.57778100 2.79982700
C 0.71534000 -1.89628000 3.82532500
C 1.85754800 -2.68775300 3.80712500
H 3.68229900 -3.21079200 2.81473500
H -0.00697400 -2.00593300 4.62187900
H 2.01097500 -3.41030000 4.59899900
O -0.56255900 -0.15667500 2.68948100
C -1.61835000 -0.31484300 3.62368100
H -1.99858200 -1.34037400 3.61462800
H -1.29389500 -0.05564200 4.63518100
H -2.40305800 0.36805100 3.30092600
H -5.12303200 1.53815500 1.16469900
O -3.23630800 4.79104500 0.70923500
C -4.54657200 5.08517100 0.20704800
H -4.57567600 6.16445200 0.07420400
H -4.70242000 4.59033000 -0.75398700
H -5.31342900 4.76911300 0.91096200
K 0.87114400 4.50035300 2.01305200
O 3.47345000 -1.43315700 0.75458700
C 4.59233300 -2.30006300 0.64457000
H 5.11333700 -2.00045700 -0.26111000
H 5.26001500 -2.19281800 1.50382200
H 4.27046000 -3.34051500 0.55420400
O -3.69291200 0.07876100 0.73783100
C -3.18754600 -1.22458500 0.47709200
H -3.99491500 -1.91269500 0.71317700
H -2.91237100 -1.32353800 -0.57575500
H -2.31931300 -1.43442500 1.10759500

SSE – K⁺ - position 2.

C -2.91358300 0.47657700 -0.01785600
C -1.59599400 0.74751200 -0.34957600
C -1.04847000 1.98113900 -0.00489300
C -1.81780000 2.94630800 0.63515500

C -3.14581200 2.67266900 0.94581900
C -3.69060300 1.43978700 0.62460900
H -0.97760900 0.00388800 -0.83238200
H -1.35780800 3.89649100 0.86456100
O -5.00881700 1.15086100 0.92733200
C 0.41348800 2.26435500 -0.27949900
H 0.67292000 1.84571300 -1.26276900
O 0.60286900 3.65981000 -0.26082100
H 1.54643200 3.84026400 -0.14883100
C 1.30423700 1.57409000 0.77168600
H 1.06355600 1.99271700 1.75513300
C 2.79576100 1.71736800 0.48299800
H 3.35291500 1.15474100 1.23786300
H 3.00812400 1.28427500 -0.50058400
O 0.99969700 0.18321400 0.72608900
O 3.13218700 3.10065600 0.52555700
H 4.07164800 3.21439600 0.36440400
C 1.21438200 -0.51391000 1.88489500
C 2.29010400 -1.40415200 1.96865600
C 0.32015800 -0.38732100 2.95352000
C 2.46702300 -2.16852000 3.12471000
C 0.50279700 -1.14178300 4.11195500
C 1.57437600 -2.02441700 4.17819700
H 3.28990500 -2.86383600 3.20923800
H -0.17552800 -1.05309800 4.94876000
H 1.71708200 -2.61505200 5.07464000
O -0.68969000 0.50029000 2.75647600
C -1.62053300 0.67770300 3.80347600
H -2.14775900 -0.25536900 4.02515300
H -1.13265700 1.04515400 4.71139400
H -2.33058100 1.42032900 3.44203700
H -5.14158400 0.22352700 0.67753500
O -3.99900500 3.56758500 1.56922800
C -3.40410900 4.77337900 2.04929400
H -4.18853100 5.32029200 2.57100800
H -2.59376400 4.54865700 2.74535800
H -3.02634400 5.37589100 1.22147000
K -6.54768000 3.11365800 1.48834600
O 3.09930400 -1.44695700 0.88442800

C 4.17568900 -2.36840000 0.90554900
H 4.67881900 -2.26192400 -0.05232100
H 4.87578300 -2.13897500 1.71391000
H 3.81179900 -3.39371500 1.01424500
O -3.58235800 -0.68644700 -0.25145300
C -2.83878200 -1.76898200 -0.80091300
H -3.52522100 -2.60967400 -0.85531400
H -2.48290200 -1.51806700 -1.80253300
H -1.99343700 -2.01624700 -0.15423200

SSE – K⁺ - position 3.

C -2.75237100 0.46937700 -0.96136900
C -1.38704300 0.77392400 -0.93174300
C -0.89962400 1.77323100 -0.09930600
C -1.78206900 2.50918400 0.69930200
C -3.14209000 2.22525800 0.65716000
C -3.63789200 1.18918900 -0.15595500
H -0.72619900 0.20431600 -1.57571200
H -1.39298400 3.32300100 1.29728500
O -4.95488900 0.88174100 -0.15131800
C 0.57712400 2.08827800 -0.04746300
H 1.04224700 1.71214100 -0.96867100
O 0.70596000 3.48748800 0.05119500
H 1.64624000 3.69247700 0.13983300
C 1.28858200 1.43058000 1.15655900
H 1.04274300 2.01335400 2.05183100
C 2.79994400 1.38866000 0.94342700
H 3.29122200 0.95177600 1.81871600
H 3.01364100 0.76469100 0.06973300
O 0.79238000 0.08786400 1.31686000
O 3.22426000 2.72897400 0.74479100
H 4.17108500 2.75695600 0.58773000
C 1.26192000 -0.58138000 2.42805300
C 2.26894600 -1.54860300 2.28802200
C 0.69963200 -0.33205900 3.68361500
C 2.71174400 -2.24387000 3.41416400
C 1.15118700 -1.01636700 4.81024700
C 2.15553300 -1.96283700 4.65631600
H 3.48869700 -2.99046300 3.33151300

H	0.73154700	-0.82230700	5.78732900	C	1.30490900	1.56472100	0.79015200
H	2.51142300	-2.50029500	5.52633400	H	1.06108000	1.95443600	1.78444100
O	-0.32605100	0.57941100	3.69669100	C	2.80136100	1.69005400	0.52086100
C	-0.66870800	1.15772300	4.95571500	H	3.34220900	1.10188600	1.26838600
H	-1.14762200	0.42496100	5.60902300	H	3.01702200	1.27580500	-0.47018600
H	0.22067300	1.56353600	5.44154600	O	0.97561900	0.18036900	0.69640200
H	-1.36700300	1.96224500	4.73690100	O	3.15681100	3.06620600	0.59775600
H	-5.42168300	1.54434900	0.37550300	H	4.09985500	3.17098000	0.45250600
O	-4.10836500	2.86402500	1.36546300	C	1.15888000	-0.55301800	1.83798300
C	-3.75098900	4.06137400	2.04615400	C	2.21778000	-1.46449900	1.91168100
H	-4.67441700	4.46073800	2.45637800	C	0.25575500	-0.43502700	2.90088400
H	-3.04971200	3.85059400	2.85769500	C	2.37091700	-2.25754400	3.05159000
H	-3.30927400	4.77883600	1.35123800	C	0.41634900	-1.21774200	4.04428600
K	-1.76107400	-0.55756900	1.70709100	C	1.47195600	-2.11989000	4.10077700
O	2.74916400	-1.71002900	1.04043500	H	3.18225900	-2.96712200	3.12894400
C	3.76613000	-2.68422800	0.84195200	H	-0.26576400	-1.13261100	4.87837500
H	3.99656400	-2.65982000	-0.21968300	H	1.59804000	-2.73009000	4.98657600
H	4.66090700	-2.43706100	1.41890200	O	-0.73840800	0.47193000	2.71623200
H	3.40945900	-3.68000700	1.11622800	C	-1.62356300	0.70357300	3.79404500
O	-3.17721700	-0.58168800	-1.71104600	H	-2.19551800	-0.19759400	4.03594100
C	-4.07091600	-0.25754400	-2.78618100	H	-1.08410500	1.04188300	4.68351200
H	-4.25593200	-1.19128100	-3.31100500	H	-2.30178900	1.48588600	3.45741300
H	-5.00666800	0.14862900	-2.40376600	H	-5.30247500	1.84869400	1.41381700
H	-3.59191500	0.45654500	-3.46015500	O	-3.99934100	3.37942100	1.70278400
				C	-3.54113400	4.64721500	2.16012900
				H	-4.38240600	5.10454800	2.67397700
SSE – K ⁺ - position 4.				H	-2.70494100	4.52496500	2.85273600
C	-2.88469300	0.49691000	-0.13284200	H	-3.23642300	5.27017400	1.31660500
C	-1.56940600	0.81443800	-0.44317000	K	-6.08108600	-0.83770700	-0.36181400
C	-1.02726400	2.01786500	-0.00443100	O	3.03747400	-1.49596800	0.83455600
C	-1.79888800	2.92667400	0.71335600	C	4.11598400	-2.41470100	0.85824700
C	-3.11878100	2.60925300	1.00155600	H	4.63582700	-2.28966800	-0.08841000
C	-3.66086500	1.39682900	0.58287700	H	4.80071800	-2.19793600	1.68307100
H	-0.93916700	0.12124000	-0.98154900	H	3.75400700	-3.44310900	0.94216500
H	-1.35229900	3.86040600	1.02537900	O	-3.50257900	-0.68656900	-0.49371900
O	-4.97946400	1.10579000	0.88162400	C	-2.63900000	-1.72673200	-0.95579500
C	0.43778300	2.31067900	-0.24376300	H	-1.83859400	-1.90285000	-0.23433000
H	0.71389000	1.94049800	-1.24211000	H	-3.25245500	-2.62212600	-1.04881300
O	0.62987200	3.70139700	-0.15047900	H	-2.21604800	-1.47509900	-1.92991700
H	1.57382600	3.87331000	-0.03052700				

SSE – K⁺ - position 5.

C	-2.32700700	0.15656700	-0.91998800	C	-4.43856400	4.01301800	0.96011900
C	-1.06031600	0.71126800	-0.74185600	H	-5.47371200	4.30949600	1.10516600
C	-0.90945400	1.92377800	-0.08963200	H	-3.92000700	3.99740700	1.92183100
C	-2.03764700	2.64694700	0.30245800	H	-3.94402100	4.71051300	0.28030400
C	-3.30154600	2.12211700	0.06823400	K	-1.12504100	-1.55968900	1.04823500
C	-3.45979800	0.85154900	-0.51288500	O	1.59207600	-1.73966500	0.75870000
H	-0.19426900	0.15151900	-1.08336100	C	2.43074000	-2.69952100	0.11674500
H	-1.90363200	3.61206800	0.77185800	H	2.22937600	-2.60964200	-0.94794900
O	-4.68677700	0.29959900	-0.65195900	H	3.48155400	-2.47826000	0.31354900
C	0.47215200	2.41680500	0.25482000	H	2.19781900	-3.71392400	0.44929500
H	1.16994400	2.07925900	-0.52446900	O	-2.40371300	-1.15029500	-1.34801100
O	0.43091700	3.82047100	0.32392300	C	-3.08300900	-1.35716700	-2.59773800
H	1.31728200	4.13022400	0.54763600	H	-3.02121300	-2.42273700	-2.80591200
C	0.96115400	1.85844500	1.61780500	H	-4.12460700	-1.04910500	-2.51827500
H	0.48075900	2.43888300	2.40776500	H	-2.57638500	-0.79417000	-3.38413500
C	2.48378700	1.94881900	1.72436100				
H	2.81042500	1.72542700	2.74361200				
H	2.92214500	1.21136100	1.03856700				
O	0.55171000	0.47536500	1.73662300				
O	2.85734800	3.26609700	1.35870400				
H	3.80449800	3.38333100	1.46183000				
C	1.23559800	-0.34336300	2.60418100				
C	1.80060300	-1.51801000	2.09441700				
C	1.31767100	-0.07171400	3.97922200				
C	2.47966700	-2.39963900	2.93503800				
C	2.00496100	-0.94830400	4.81790800				
C	2.58042100	-2.09618100	4.28580000				
H	2.92988100	-3.30241600	2.54673600				
H	2.09052500	-0.74517800	5.87595100				
H	3.11288700	-2.77303800	4.94196100				
O	0.72151200	1.07235100	4.37604300				
C	0.80943100	1.42769500	5.75089300				
H	0.32954300	0.67277100	6.37830400				
H	1.85176300	1.55645700	6.05285300				
H	0.28127300	2.37236600	5.84735600				
H	-5.34254500	0.94434100	-0.35355300				
O	-4.47924200	2.70960100	0.39301200				