

Supporting Information

Inaccessibility of the μ -hydride species in [FeFe] hydrogenases

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1 Computational methodology

The structural model was cut out of the crystal structure of the [FeFe] hydrogenase from *Clostridium pasteurianum* (pdb code: 3C8Y).¹ The oxygen atom of the bridging dithiolate ligand in the [2Fe]_H subcluster was replaced by NH.²⁻⁴ The extraction of the QM region leads to dangling bonds where the connection to the protein was cut. Hydrogen atoms were added at a distance of 1.096 Å to saturate the generated dangling bonds in a way that the bond direction of the original bond was retained. The added hydrogen atoms and the first carbon atoms of the QM model were kept fixed during structure optimization. This procedure maintains the directional constraints imposed by the protein matrix. In addition, the backbone atoms (C_α, C, O and N) of residues 232, 324 and 325, which are contained in the model, were kept fixed during structure optimization. The capping hydrogen atoms of the backbone parts were allowed to relax during structure optimization.

The structures have been optimized in vacuo and the gradient convergence criterion was set to 10⁻⁴ hartree/bohr for the length of the geometry gradient. Single-point calculations were performed with the COSMO electrostatic continuum model⁵ and $\epsilon = 4$, as is often done to model the screening effect of a protein (see, e.g., Ref. 6). For iron a modified (COSMO) radius of 1.391 Å was chosen, as suggested in Ref. 7. The SCF convergence criterion was tightened (10⁻⁷ hartree) compared to the default value (10⁻⁶ hartree).

Frequencies were calculated from the analytic Hessian of the electronic energy with the aoforce program of the TURBOMOLE program package. However,

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aoforce does not allow for a special treatment of frozen atoms. Thus, some normal modes always feature imaginary frequencies originating from these structural constraints. Because of the frozen atoms in our structural models, some normal modes always feature imaginary frequencies. These imaginary frequencies are generally low and well separable from modes corresponding to transition states. As a consequence, only differences in energy and not differences in free energy are obtained, since the imaginary frequencies would introduce significant errors in free energy calculations (apart from the fact that the standard quantum-mechanical rigid-rotor, harmonic-oscillator, particle-in-a-box model is rather poor for enzymatic reactions). The modulation of reaction energies and barrier heights calculated from electronic energies is usually small and can even be on the order that the standard approximation introduces (the rigid-rotator, harmonic-oscillator, particle-in-a-box approximation) applied in quantum chemical calculations may become inappropriate for the condensed phase and thus at the reaction center of an enzyme under physiological conditions. To calculate the energetics of enzymatic reactions from electronic energies has thus become the standard approach (quantum mechanical cluster approach⁸).

The antiferromagnetic coupling pattern was enforced by exchange of iron atoms after the first converged SCF procedure (see e.g. Ref. 9). The two iron atoms of the cubane proximal to the $[2\text{Fe}]_{\text{H}}$ subcluster were coupled antiferromagnetically to the two iron atoms of the cubane distal to the $[2\text{Fe}]_{\text{H}}$ subcluster. If there was spin density on the $[2\text{Fe}]_{\text{H}}$ subcluster, it was coupled antiferromagnetically to the two proximal iron atoms of the cubane. This coupling pattern was investigated in detail by Fiedler and Brunold.¹⁰

The calculated frequencies were not scaled, as the scaling factors for the BP86 functional in combination with a proper triple-zeta basis with polarization functions would be close to one.^{11–13} Reduction energies are calculated as difference in electronic energy of the optimized structures with the charge of the product increased by -1 .

2 Effect of the H cluster surrounding amino acids on intermediate **3**

The effect of the amino-acid residues surrounding the H cluster, especially the effect of the salt bridge from Lys358 to CN^- at Fe_{d} , can be illustrated at the example of intermediate **3**. The structure of intermediate **3** is shown in Figure 1 (top structure). The CN^- forms a salt bridge to Lys358 (as discussed for intermediates **0'** and **0''** in the main article). This salt bridge leads to a high stability of the conformation shown in Figure 1. Optimization of a model of intermediate **3** consisting of the H cluster only leads to the structure denoted **3**_{small} in Figure 1. In contrast to the large model, the cyanide ligand is in the apical position and forms a salt bridge to the bridgehead's ammonium group. For the small model a conformation of intermediate **3** which resembles the conformation of intermediate **3** of the large model (**3'**_{small}) is obtained by swapping the two

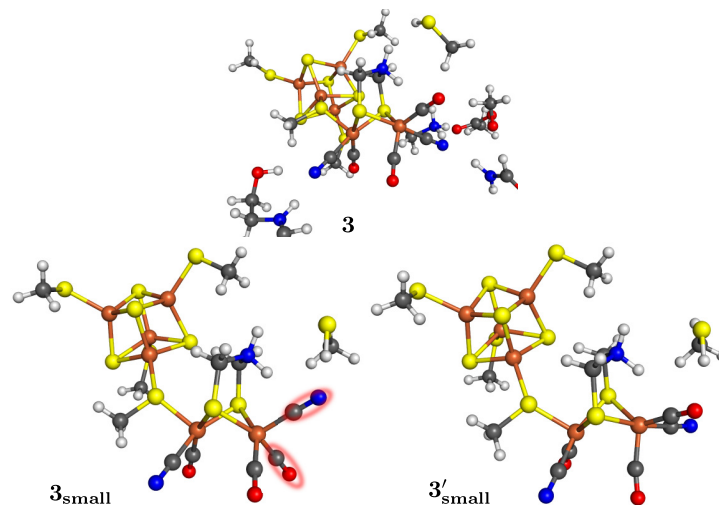


Figure 1: Top structure: Most stable structure of intermediate **3** obtained with the large model. Bottom left structure: Most stable conformation of intermediate **3** with a model only consisting of the H cluster (**3_{small}**). Bottom right structure: Conformation of intermediate **3** which is obtained when exchanging the two ligands marked in red of **3_{small}** (dubbed **3'_{small}**). **3_{small}** is -4.0 kcal/mol more stable than **3'_{small}**. All structures were optimized with the BP86-D3/def2-TZVP. Electronic energies were obtained in BP86-D3/def2-TZVP/COSMO($\epsilon = 4$) single-point calculations on optimized structures.

ligands marked in red in Figure 1. However, this conformation is 4.0 kcal/mol kcal/mol less stable than **3_{small}**. Hence, the salt bridge from Lys358 to CN^- at Fe_d is crucial for interlocking the conformation of the H cluster in the enzyme.

3 Additional reactions of the terminal-H species

Two pathways for μ -H formation are investigated in detail in the main article which we consider most likely from a chemical point of view. In order to investigate whether other reaction pathways are also possible for μ -hydride formation we explored additional reactions. Due to a lack of other proton donors in the vicinity of μ -bridging position than Lys358, direct protonation via another pathway than protonation by Lys358 can be excluded. Thus, only reactions of the terminal-H species (intermediate **4**) remain to be investigated. A possible reaction would be the shift of the hydride (as proton) to one of sulfur atoms of the dithiolate ligand accompanied by the reduction of Fe_p and Fe_d . This reaction is endothermic by $+17.5$ kcal/mol for the sulfur atom distal to Lys358 and endothermic by $+14.3$ kcal/mol for the sulfur atom proximal to Lys358. We estimated the barrier with a reaction coordinate scan to be about 28.3 kcal/mol for the latter reaction. The barrier is approximately as high as for the iso-

merization of terminal-H to μ -H but the reaction is endothermic. Hence, this pathway is unlikely. Insertion of the hydride between Fe_d and the CN^- ligand to form HCN might be possible as well. However, all structure optimization of the HCN product converged to a terminal-H structure which shows that this reaction is not possible. Finally, we scanned the position of the hydride on a grid around its equilibrium position with single-point calculations to identify possible other low-energy routes. Figure 2 shows plots of the electronic energy surface for the nucleus position of the hydrogen atom shifted away from Fe_d . Displacements of the hydride lead to a steep increase of the energy. Hence, hydride abstraction reactions seem unlikely. Reactions involving cleavage of the hydride were also excluded by other authors, see e.g. Ref. 14. By contrast, in the rearrangement reaction from terminal-H to μ -H — as described in the main article — the hydride is always bound to Fe_d . Thus, it can safely be assumed that this rearrangement process is favored compared to reactions which involve hydride abstraction.

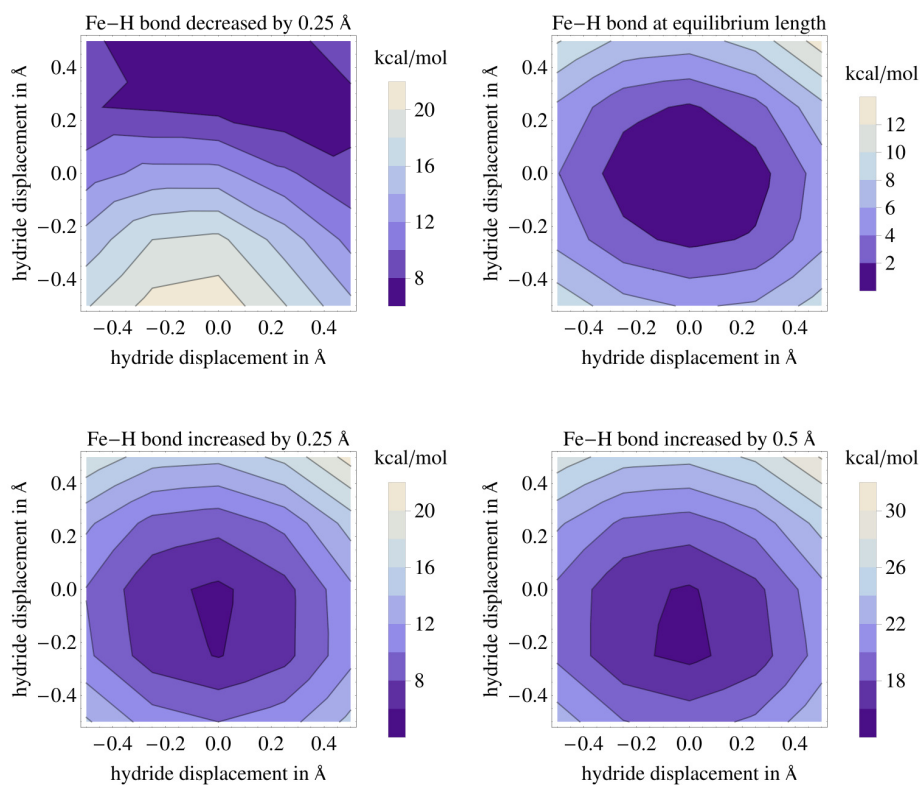


Figure 2: The hydride position at intermediate **4** was changed in the plane defined by the two sulfur atoms and the CO's carbon atom in the square plane around Fe_d. The position of the hydride was changed with a 0.25 Å step size. The scan was performed for the equilibrium bond length decreased by 0.25 Å (top left panel), for the equilibrium bond length (top right panel), for the equilibrium bond length increased by 0.25 Å (bottom left panel), and for the equilibrium bond length increased by 0.5 Å (bottom right panel). The energies are given relative to the energy of the equilibrium structure. The single point calculations were conducted without COSMO.

References

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4 Coordinates

Table 1: Coordinates of **0** in bohr.

39.96871066653503	39.94067215480364	29.65514515782597	h
50.18937057989390	38.71894591280600	52.88982453462290	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.75286600014575	37.20009835190818	31.46548019227129	h
37.17053899371361	20.91282292550184	48.81932250699352	h
32.44612638730704	20.85411360499304	50.80557781878417	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.25998755112730	44.91554228437819	49.78053148257580	h
47.90199127553674	26.81388345620934	42.58463243720755	h
46.89984873645066	42.98589706946940	46.40540489240218	c
47.54172479975625	40.96585243189991	44.76801215826203	o
36.32115079980820	30.52638448623426	40.18778406522960	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.03674982512219	27.72334954315837	42.64847936271135	c
41.57704676901798	26.83555956545806	42.04819897871137	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.56449802687524	19.19665093054746	41.80537599600036	s
42.42721621695826	32.24586835777898	45.60608877741405	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
42.86384721314889	28.25728724989586	48.22808806569056	fe
37.06171075504647	37.14756047536596	38.45246355859442	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.56855875600097	26.48661675105979	34.12915240482045	s
39.28063421731346	33.42848975239998	38.72502130602587	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
33.96917970775633	34.02814701683767	38.88787843413800	fe
36.17151287603395	30.23261319084859	36.02490631247039	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.23690076205991	21.02031310241802	51.43507535091554	o
42.80487827686928	37.78558142083922	42.54164006067941	h
40.55716452331566	21.98731759537789	56.13767708458050	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.09654956451383	24.75820358755269	44.04337465489877	h
47.56322864995717	39.43043024460322	49.54336882631011	h
50.67184464350142	43.45627630531236	47.95445019498292	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.72617689954333	24.63264419300691	57.11712141479680	h
36.65125829280161	35.37580911218657	34.64552069472295	fe

41.11729264671375	21.21226671676301	45.18376353189745	h
41.58838356703429	17.93643423906952	45.71299254675547	h
43.70753463839568	21.71790222829937	41.27634055874318	h
39.82909178975406	32.33551704775352	34.71042654513239	s
32.95458102081582	33.00278764053591	34.99305943837692	s
46.41727200042914	27.64909827219607	52.40065743793732	o
39.21741644463587	25.19688728141235	36.68408356794950	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.88112046942734	22.60198943171294	34.98464466698344	h
34.52321240311288	37.53967649503476	43.24363351470394	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.83822084567145	35.55536052676621	41.26586344485550	s
32.00360685624286	37.13955405910332	45.42804846083263	h
33.67390739277011	28.86528164504192	44.87087723006621	h
35.72079220977878	29.56638969356752	47.45016297266950	h
32.32325068036502	24.96861689679742	47.72454422104426	h
35.28580296556277	25.55918317156734	49.13766193191631	h
35.17096262065407	24.94812440082500	46.10617366733444	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.18681580338885	25.84669022077760	47.51134659037393	n
34.65980481445451	18.70948534020942	48.25603964815102	h
37.33948342116821	24.34987404528601	54.20564499561366	h
25.22293841516336	20.42075829467269	46.92780166873828	h
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24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.45348297187170	22.21802063768454	48.66140228812919	c
29.42322704477073	24.25483556877654	47.83201281696851	o
29.58985354629730	20.39001717715242	49.69466889343686	o
45.90680462452012	36.53054526231450	42.22149996996753	h
39.60339958388850	36.85038530007687	28.32560284926011	h
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44.02305980785066	36.59076695825087	41.36988432835967	c
42.77557036527961	33.37418127441806	41.35595249238138	s
44.08952844473031	25.80998140288952	42.40961474087096	n
46.06509243447299	29.62646172759522	45.62266857671307	s
40.24225922799756	25.30162181717463	41.62732348447755	h
40.19217199386696	28.50969815035984	44.80476241411631	s

39.65631372999698	34.04227384544674	45.79268927176581	c
37.84374293857959	35.26938525056570	45.93207159194036	o
44.43033953575986	34.99438332731451	46.74112787155214	c
45.62342152522351	36.74831538458184	47.42794983968216	n
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41.20324431505838	32.61819106001089	51.12481512779348	o
40.20222779580156	26.62805249873649	49.92642298920538	c
38.45193834629191	25.62884618944680	50.88012205412124	n
44.99358373227091	27.90111842226606	50.73372610635681	c

Table 2: Coordinates of \mathbf{O}' in bohr.

39.94757438515317	39.94387356213088	29.64923234442961	h
50.19097031879298	38.71681582444723	52.88552204309801	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.76464881363966	37.21315843085436	31.45995855177068	h
37.17107994806837	20.87998367676424	48.77476600634485	h
32.47527447386648	20.90857458964575	50.83827399119436	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.23158740545367	44.91300431745772	49.77024452108975	h
48.16632090274503	26.77143342373707	42.69103977605879	h
46.91791082950392	42.95345233019520	46.39042229637241	c
47.58555538523696	40.92609405349568	44.77241214640722	o
36.37028074956476	30.51593939117901	40.20835247785104	s
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41.12531597326299	19.35042135416161	44.26975977401633	c
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36.20305756819735	30.20099554819827	36.02396326848942	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
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32.98131529054312	32.96986772606885	35.01531404788701	s
44.97192259173102	22.33564804391077	48.56028705026737	o
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31.89788723985617	39.64433382965327	43.16796440546944	h
37.88502973956133	22.60138764694585	34.98572244044804	h
34.52787457634366	37.54666315996590	43.26081834408011	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.87164252324618	35.55517052256224	41.23952636500981	s
31.97740845645877	37.13201353316357	45.41884327561068	h
33.65341170803219	28.82703625555961	44.86828180185289	h
35.72017964477922	29.57870656878132	47.42937557157018	h
32.33960709713703	24.97715584392226	47.74546845457557	h
35.25447931389511	25.66147813237704	49.23488376806490	h
35.23110502777362	24.94152007134264	46.21302640504728	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.19251441060349	25.86280006360916	47.56272976838709	n
34.62717252475422	18.70243676280947	48.28395042467151	h
37.35183399926485	24.44866762733303	54.22450454128057	h
25.24506525866121	20.42992886753067	46.91137375263438	h
24.74974352479390	21.19460121251243	50.13454404515027	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44961870225784	22.23801608001154	48.68548202108197	c
29.41504217772137	24.25568553244464	47.80970251710158	o
29.58578889984594	20.44355852777798	49.77770698054346	o
45.92201734566825	36.42426832879956	42.17206582920247	h
39.60263513297916	36.84967455518400	28.32505575464967	h
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46.22264371623558	29.16246637929394	41.23577639391403	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.16112264409662	37.80279431540961	31.20160210728468	s
44.95737721125589	42.74923789521419	47.09697824820888	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.99423545569216	44.70539624810819	45.26253237399334	h
46.95933320194218	39.32758205340356	45.55817084144213	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.60016850575512	33.44938861979472	41.50236220288267	s
44.38882841432403	25.81573555772209	42.21149455843855	n
46.17732355267537	29.43464837872463	45.81236456483970	s
40.55303885825788	25.26315163197430	41.46924633334180	h
40.49834268231263	28.39061674956972	44.77070694785105	s
40.15618476662372	33.43557754492905	47.21831900213851	c
38.53107060095834	34.37207752656168	48.37547128350414	o
44.62879494984033	34.85815590233639	46.72190207018259	c

45.78679178311585	36.63679643203254	47.42056780716733	n
44.44748406117507	28.65249734402447	51.08525020989363	c
45.30841742844269	29.32854786587638	52.99407638801467	o
40.06615922414726	26.76102551240369	50.00460956718640	c
38.17570481697142	26.19747124057551	51.04379157988026	n
44.16089341064031	24.38999934898510	48.35043203384059	c

Table 3: Coordinates of \mathbf{O}'' in bohr.

39.92227899191835	39.94879201839215	29.64087596456576	h
50.18996062710941	38.71675723048578	52.88642492927488	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.78845804417333	37.23111557101721	31.44705886073341	h
37.14411534382394	20.61505623339748	48.49663066177047	h
32.73916348392292	21.34166024839535	51.08515682366830	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.22362043089815	44.91273272792097	49.76960039798017	h
47.75724392293354	26.34192700989987	44.82402416255057	h
46.94501923061565	42.98311839989825	46.36928775414758	c
47.64064288670377	40.98994735693928	44.71963881134401	o
36.39032415845443	30.44732404650506	40.22915633352887	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.00887994108796	27.36243645731758	44.36413238219323	c
41.67254809585595	26.65323861771471	43.05393131261753	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.37170511062381	19.72046364914506	41.64240539212861	s
42.39993833582047	32.47871925760367	45.74446312195226	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
41.92967934273319	28.47448312013764	49.29742569337434	fe
37.14757588630422	37.07609748767962	38.52589669374321	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.56883236878289	26.47702394864819	34.11863949361562	s
39.33226411194745	33.35413358336542	38.79709084128058	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
34.04336613291582	33.97449353284077	38.93307656919295	fe
36.24032792078949	30.18636471880762	36.03587543135346	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.61342802016442	21.43637761467514	51.39437126081519	o
42.92216126911650	37.86640260369120	42.57173588406945	h
40.55026803919418	21.98523264049576	56.13243552921994	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
43.66986633550241	24.62201459447170	45.61293738992211	h
47.55804772010335	39.42780878487868	49.53225664625116	h
50.68109365514277	43.47747257549619	47.99027646215789	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.68711523740027	24.56009203374551	57.10111420305806	h
36.72887283811227	35.31804172556299	34.68816046868251	fe
41.07308103384273	21.04907619819621	45.45212685714174	h
41.72290971964951	17.78823699703153	45.49386501180756	h
44.08906530860705	22.15654068934400	42.20383871206630	h

39.89921691966025	32.29282919903640	34.75985278936611	s
33.02600298389163	32.96600404283038	35.04385912768328	s
37.14028989617567	28.54994206214513	52.00487738955820	o
39.21300609727233	25.19649335015663	36.69045473782875	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.88766588120264	22.60111261959686	34.98794051003346	h
34.52897181475053	37.55158540903640	43.26757029879526	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.88264761087334	35.53838538235103	41.24938763909017	s
31.98097888772497	37.13902571713398	45.42198576361283	h
33.66644143832659	28.81899260462709	44.86520244455225	h
35.71277263213714	29.57439701302121	47.42369941884080	h
32.25632668467916	24.91004869433127	47.41651341375265	h
34.78058359435757	25.52669558009114	49.34232611767812	h
35.41500951360180	24.97036237507684	46.36013697976095	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.13805209169345	25.84502551935599	47.52838391906866	n
34.35406014316762	18.69319997238435	48.56468065287228	h
37.10866289380041	23.96859833063885	54.20451157581029	h
25.33426551139173	20.48387989378026	46.84323142975194	h
24.72883390930321	21.13832308348096	50.09730151770523	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.45472996775512	22.36274703899845	48.74008245799904	c
29.45664702956043	24.02964697931577	47.31257479082281	o
29.56640149026170	21.04211602515388	50.38755559460057	o
45.92578338455707	36.45514533015881	42.17225708742643	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.98881898516451	27.74477347632205	41.31279918039777	h
46.28518059143260	28.52041334656231	42.66164215104968	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.17897747623308	37.77029202987556	31.24462674932374	s
44.97769817841174	42.75260480342441	47.04661615606018	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.02582168472432	44.75762152346672	45.27711874182100	h
47.00075674484545	39.39412461141410	45.49673246871691	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.60749323079472	33.44369375069602	41.62813802859574	s
44.01204448612738	25.56224873685172	43.94213517085327	n
45.57741461040065	29.65905034472593	47.05065349931200	s
40.31556700587844	25.13695737918590	42.64859626822177	h
40.06366359767327	28.84586413331914	45.29142407797764	s
39.86448475560952	34.12549131120046	47.12905825351318	c
38.22571410604112	35.28831258946992	48.03929753243582	o
44.46007040379322	35.17996789201497	46.84871578635982	c

45.71641177354132	36.90336892864907	47.51275125923856	n
43.56716316644830	29.21291413646935	52.09782361768700	c
44.63749474890701	29.68598743977942	53.96323886116896	o
39.04983711482161	28.60300340703530	50.87537684460381	c
42.00974357783323	22.66155912529280	49.65928726095488	n
42.06007927444175	24.88667423005447	49.52713055125368	c

Table 4: Coordinates of **1** in bohr.

39.90706258350838	39.95184658811364	29.65055909083754	h
50.18450286234414	38.72150951358698	52.89596491983819	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.77786762963311	37.23827665012691	31.46005079107621	h
37.17131301416602	20.82569095310835	48.70143778241832	h
32.52757069480166	21.00850976683938	50.85584811618722	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.46293024269100	44.92029594746749	49.82935151247487	h
47.99931429640990	26.71747953549564	42.57924907928459	h
46.68792674902767	43.11180260146120	46.58528934433662	c
47.03399064620142	41.06811607903980	44.87756370430705	o
36.32845938644753	30.58259626117274	40.21944904185951	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.20066850598319	27.74917844564807	42.62133159490376	c
41.58266604171636	26.88423035533264	41.90425301649372	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.30126070674432	19.64900490519572	41.55866772984449	s
42.45188960680944	32.10484323276042	45.42585244796516	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
42.96171636529581	27.89115405279794	47.96718560075954	fe
37.18459578454681	37.09384564766668	38.41604146152866	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.54964093518245	26.47396740861010	34.13837695873788	s
39.30712624155453	33.39007515591570	38.78873463788433	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
34.17070544397438	34.05714528076960	38.82989906933820	fe
36.12646764993780	30.19216089097315	36.01393059578087	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.34654194365274	21.15105448676146	51.41285789402784	o
42.84338096458480	37.79568876321633	42.56897784163487	h
40.55492824112170	21.97723112061434	56.13831841893477	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
43.90328315499258	25.28926299727775	44.52398042036499	h
47.56975360784665	39.42903145334542	49.55958949261532	h
50.61004546736405	43.35057482830859	47.77664416753097	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.74308594565935	24.65796869041442	57.12833838617745	h
36.66358618637259	35.31774222021380	34.56663863980746	fe
41.09470735227311	21.08370702212938	45.40798257499329	h
41.78380601372452	17.77188001558867	45.43237057326793	h
41.56350759700129	20.40985670799965	39.84353595474887	h

39.80728467610465	32.25300749032741	34.77591748699113	s
33.01361671217381	33.00566570548212	35.02974676247907	s
45.25892326550774	22.97023940865083	48.97897789109067	o
39.22095873308255	25.20674633218625	36.66416772929433	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.87227638035071	22.60629620530980	34.97471907799353	h
34.53866267729333	37.55682628538462	43.41538882830311	h
32.47305373188985	37.67924920624719	43.47692895772752	c
31.04958076389948	35.58910237677298	41.10440871125162	s
31.84025760392369	37.08309286171727	45.36227446011080	h
33.67416972151925	28.85684116682913	44.87085784187096	h
35.72366407788905	29.54224806271556	47.48028901311732	h
32.19300311101951	24.99020354852151	47.69277732225559	h
35.13210251925531	25.60556548744553	49.22093518896040	h
35.13537078090627	24.90083019860013	46.20623914689292	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.10674977693484	25.85018226824489	47.54206409429039	n
34.57390929940691	18.68531802531700	48.34021761731414	h
37.32457842873144	24.39171220032697	54.22161318060557	h
25.24756808275572	20.42771416769222	46.91582633960622	h
24.77261530533288	21.19740626827407	50.14410060879673	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.44912595011321	22.27770863763471	48.65683761654578	c
29.38846722811688	24.27954782790734	47.68971341823595	o
29.63248879610748	20.55683117192136	49.80629235291082	o
45.90604868259560	36.47766604737501	42.22159555144632	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.76092898464859	28.16919625053488	40.28270216570406	h
46.00522843108454	28.97068969274030	40.95368664826053	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.16164009422241	37.76493246395881	31.19198450904117	s
44.79990534561010	43.03610892842065	47.48665149388940	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.77525619832469	44.86460766578239	45.46347806643887	h
46.46739576488710	39.48610350073809	45.71894685963052	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.72274170253298	33.39603812691178	41.39936087772757	s
44.11875667527364	25.83399613619224	42.58446627616915	n
46.07022422629458	29.68641349903860	45.50424810503170	s
40.35154568560220	25.29094511294194	41.40349480825103	h
40.25290052463585	28.52241163072314	44.65987339946440	s
39.75737475877826	33.70135453521432	46.46918912575649	c
37.99308834449955	34.82911880936127	47.14988537973927	o
44.34884142076937	34.82401931286587	46.81326873637198	c

45.47914999900529	36.60787115117397	47.52672771176665	n
43.91431033262508	29.76709321149407	50.57086304831167	c
44.51055933285251	30.88773751881086	52.35880924566253	o
40.05968450617471	26.94927993765268	49.79341549737376	c
38.25051900333631	26.26139251359628	50.89262915319633	n
44.30425854121773	24.92125823007927	48.51761137802026	c
44.53086823195120	24.21334836856480	41.56051859370863	h

Table 5: Coordinates of **2** in bohr.

39.86550906932277	39.96163812501639	29.63383492295196	h
50.18551979131814	38.72021940254938	52.89232550572605	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.81699518243870	37.26519818666974	31.43745744561616	h
37.17096426849932	21.01032619554276	48.96385247689395	h
32.35876564883519	20.70391307651310	50.61677155216560	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.28486351826432	44.92040742930136	49.78283639396901	h
47.92115865038991	26.90081067220600	42.61949169137408	h
46.86412249157463	42.98136402822649	46.43166503881454	c
47.44223897518989	40.91821485805941	44.82752561195316	o
36.34112639758646	30.49437944685234	40.23050456192303	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.11145777677385	27.90971236886144	42.73306786210922	c
41.49194610541505	26.98217852816664	42.12936362353613	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.27435129983814	19.70490683942119	41.54749572477420	s
42.40278700308750	32.25389949009116	45.58910689129356	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.00079378560793	27.95040661825460	48.14769715729721	fe
37.09977581314504	37.20117484513931	38.45385050716587	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.62676123397200	26.56355766398087	34.16288608621211	s
36.72961269650219	35.26018238126701	34.76214088587744	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
39.17201269464997	33.45321082953703	38.73771991547326	fe
34.12726761046917	34.01329098780811	38.83718210682007	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.08787322076494	20.86475825576595	51.40396146609547	o
42.88893434042153	37.83969570707317	42.57083039516254	h
40.55226970303312	21.97852870047579	56.13639975846672	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
43.88276515743119	25.44992646616500	44.74301503038872	h
47.53838911542930	39.43443030631705	49.56001680909265	h
50.66472411221336	43.43943705177877	47.92877500306450	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.76311741710400	24.69296682149825	57.13487807979616	h
36.28504762444758	30.32810995690647	36.07867761062767	fe
41.09416979998730	21.06590132172043	45.43615453392288	h
41.80508687496434	17.75507776932289	45.39755976256647	h
41.56317769812325	20.71864264631197	39.93573435561747	h

39.96840698439552	32.33175052998573	34.77696286244673	s
33.02131824731446	32.97206209489337	34.99281717250766	s
45.70792575636601	23.25600250058152	49.23478771594812	o
39.24692787735773	25.14333818876497	36.68803499811353	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.83488810638336	22.60257612449767	34.96048927993752	h
34.53563154641125	37.55325608825971	43.34488490654685	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.96114048266770	35.57096738672445	41.16331348623405	s
31.91274025718513	37.11074412163491	45.39557086286375	h
33.65068237628785	28.80809009038693	44.86833608092471	h
35.70865675509716	29.60408711010826	47.41696384408221	h
32.37108160374576	25.00158209577967	47.87172907810898	h
35.17105665783185	25.68262528629012	49.21722950621435	h
35.17294902503374	24.92293698205007	46.21054462728993	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.21588453664160	25.87157833837077	47.59937737147859	n
34.78789333218045	18.73839432312245	48.14917751000774	h
37.39195643088446	24.47069686105133	54.22992424024935	h
25.13256453229096	20.37153197990757	47.00797663948447	h
24.83705609893931	21.29297182254885	50.20978837348450	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.46721398149064	22.17962355209058	48.54932465033122	c
29.40742470031040	24.32584954682005	48.03094306403846	o
29.64518185589283	20.21087060161251	49.22504390038610	o
45.91680497813317	36.44980207849503	42.19453582351245	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.61538600540458	28.25126437092329	40.49091250059062	h
45.82951322239331	29.14384257844349	41.08367332414976	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.19357037765014	37.66300267246098	31.25936242497664	s
44.91519874382412	42.83642001344364	47.18196473493440	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.96422942634815	44.72108268560915	45.28522324425496	h
46.73880570260960	39.35417339236756	45.62580141753841	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.62570183798862	33.43853921088792	41.43718353676626	s
44.05521080351531	25.96641429047376	42.76864764207949	n
46.03538874984482	29.85051218568519	45.61345150865289	s
40.26389452945364	25.37176568685401	41.67211080270578	h
40.22033591891109	28.64933709124680	44.89356419845496	s
39.69136864922962	33.88850022883923	46.45693074579021	c
37.90680797685949	35.04307512172330	47.05777420351858	o
44.32166893332441	34.98356428466352	46.88487372859223	c

45.49385782162410	36.76456543041524	47.56153899933777	n
43.74722894487771	30.04830284303831	50.63988134322982	c
44.25806606952623	31.24397535214801	52.41964353732237	o
40.15396313719123	26.80063943719367	49.91303973205869	c
38.34277318748229	26.00327489410157	50.95053313613258	n
44.58130194277340	25.11446758466611	48.72879130022598	c
44.47684994924666	24.35882305712736	41.73834604162391	h

Table 6: Coordinates of **3** in bohr.

39.97670640666703	39.93440672428501	29.65773412455072	h
50.18397864890979	38.72098565957179	52.89606692573433	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.73348223840775	37.19453061891799	31.47614177515523	h
37.16652962368272	20.83909625717193	48.71857833731959	h
32.52426860410367	20.99197502183240	50.85484404485775	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.43225845049739	44.91858188345527	49.82347536558421	h
47.94909251028933	26.99466189108976	42.35513541241575	h
46.71844199911914	43.10428201727977	46.55422054583995	c
47.09995451849890	41.06653640731528	44.84713133897553	o
36.25578694038215	30.72203801201247	40.23370771903505	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.05710190011653	27.84538028779317	42.36262050453792	c
41.64280758333483	26.81171820062303	41.74415150724482	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.59613761102646	19.06341492347775	41.85925687341803	s
42.26221864811204	32.14777450235209	45.46094004951123	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.86843644187532	28.11285794308362	47.90153071445691	fe
36.93519386242354	37.23231738218193	38.41562882147247	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.58476289428956	26.55800425325978	34.19731487426766	s
39.18700494800556	33.58211281380245	38.82604310654121	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
34.11849992715040	34.09032253697915	38.75950549377830	fe
36.03841363367446	30.26239167523198	36.06420236283662	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.33324104381936	21.13305798192477	51.42685305701322	o
42.88471403716949	37.82115925424435	42.58095246397819	h
40.55963246199472	21.98784395833249	56.13854725674950	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
43.43321333848115	25.31868320180927	47.48511906651137	h
47.55408307494606	39.43882139301230	49.56472259467149	h
50.62039972534075	43.36481648252889	47.80406469545919	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.70585704172664	24.59340160530032	57.10967587085928	h
36.47505413264791	35.46097478730800	34.56858921711776	fe
41.15530053500007	21.22768947306409	45.15166985724201	h
41.55727534284958	17.95707630240697	45.74173185605796	h
43.48168660929429	21.45304669509638	40.93752855154637	h

39.70506786668150	32.45146269511648	34.82919733001393	s
32.97632935320188	33.02418009705382	34.95908606262597	s
46.55196949349574	27.18871665471939	51.88252578997380	o
39.25086762198790	25.13822297723976	36.65618380877842	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.79733590136544	22.62122353845212	34.93113637724771	h
34.53402724329010	37.54408770339745	43.43344294007529	h
32.47242634281635	37.67852166168906	43.47608991932802	c
31.06743432051065	35.61246896314688	41.07590647734271	s
31.81624245152221	37.06502567331997	45.34710378591534	h
33.68850751903464	28.89895747638521	44.87379826719286	h
35.73358345251915	29.51306065465519	47.49609060463709	h
32.15560037796195	24.98271087080806	47.63652550271752	h
35.13034367788155	25.50376548972142	49.12540658606254	h
35.08507041275162	24.90931183114670	46.09732836280480	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.08561596849586	25.83222285263890	47.47454202419721	n
34.57751709159017	18.68938167794682	48.33428488872622	h
37.28495382274379	24.27881726820702	54.20057354115481	h
25.23369199904262	20.42005769853403	46.92571979091174	h
24.78659708684609	21.20775539930859	50.15362114835935	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44802228834708	22.27794823162134	48.63184188563429	c
29.37509526320078	24.29330737060933	47.67157686119512	o
29.64027671434678	20.55135652286753	49.75542607715841	o
45.91527213338887	36.43607329256468	42.19016498414403	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.55262849639848	28.14577112925937	40.15031949831916	h
45.90090130504777	29.20692059925882	40.79899310375871	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15960195896132	37.90504807489208	31.18368158103393	s
44.81695576095366	43.01590498325290	47.42557249225598	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.81449128508824	44.86166473335983	45.44023980713296	h
46.49063102641414	39.49146013280110	45.67129184413888	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.67223686429352	33.42147686940737	41.35781934934821	s
44.18265469315624	25.89026756087607	42.05871027261602	n
45.95609305235544	29.74463560269403	45.34711825643252	s
40.36347228735853	25.22633642905447	41.34218709433270	h
40.19091362618110	28.42701121778524	44.52221346953284	s
39.43207430518655	33.82337585819736	45.86886861935035	c
37.58139641284254	34.97463227990369	46.12870502451656	o
44.18429132531209	34.92552147365564	46.72443879526566	c

45.33597944550975	36.69019855821943	47.43702149857805	n
41.85577958378992	31.19475735109554	49.35088028561585	c
41.26031912342921	32.34347201613092	51.14270965722230	o
40.14587968476248	26.64360527389706	49.67833752701556	c
38.40080284153069	25.74612385351030	50.71958319724352	n
45.07550188980679	27.61361086808047	50.32025347997050	c
44.24140628314765	24.74970157247894	43.63247645745226	h

Table 7: Coordinates of 4 in bohr.

39.96345001955391	39.94158540661061	29.65247508556046	h
50.19001340981236	38.71867480562428	52.88950328577613	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.75628832898343	37.20346008815720	31.46369002849183	h
37.17196379102468	20.91728444675324	48.82620074218664	h
32.44153329881475	20.84699859441415	50.78769977609787	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.25426649292949	44.91496157296800	49.77831106841827	h
47.88362640933575	26.72069652751993	42.59748808451521	h
46.90179417676767	42.97427088720901	46.40436153657650	c
47.54509629666431	40.94298255484631	44.78060753262386	o
36.34368104983988	30.53146734294274	40.21687710077255	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.02000333666327	27.63540367800267	42.61110727734557	c
41.56759210399332	26.76038506002054	42.02957154609786	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.54647755202389	19.20835289220538	41.78292215256867	s
42.41773368087793	32.18091978399401	45.57105722084415	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
42.87630056135072	28.19644746149748	48.13295669136307	fe
37.07248664563884	37.16141413100418	38.46726176132623	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.57173660480147	26.49694669929149	34.13695768802510	s
39.29549205283870	33.44106723518007	38.73064626305115	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
36.19244090893802	30.23255897120324	36.04690212211730	fe
33.98111974429089	34.02804708365530	38.90264841400531	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.22703785492585	21.01225158390390	51.43229532419775	o
42.77202433671910	37.76708927581132	42.52605872434334	h
40.55478503924865	21.98178961350246	56.13752127920294	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.04212840505214	24.79248646800928	44.14577677145596	h
47.56761624506429	39.42924336590373	49.54432438836163	h
50.67227162074586	43.45770590759579	47.95704981404013	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.74437530878134	24.66070507475250	57.12764681918679	h
36.65093878480155	35.37908426222638	34.65957062804451	fe
41.12622344323004	21.21287245288687	45.18270283505763	h
41.59232918438087	17.93650357372891	45.71173558455330	h
43.79831949665039	21.75086001611853	41.38214859782781	h

39.84086578894055	32.34204684159345	34.71514277658392	s
32.97084035230112	32.99290999288005	35.00944871866284	s
46.43396055424529	27.51266630580193	52.27517046091026	o
39.22236822411107	25.18762264275621	36.68258261531425	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.87308244827950	22.60266559456785	34.98028836326044	h
34.52282965547707	37.54131100300964	43.23957102089599	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.83609872964341	35.55714363017317	41.26492914622198	s
32.00539019041636	37.13856285527238	45.42805227267579	h
33.66937126000315	28.84676298237079	44.86927727081874	h
35.71956130531043	29.57167707748548	47.44414542170199	h
32.32510983058602	24.98459981989562	47.77263186019901	h
35.29044952330536	25.61310016420449	49.18115672227986	h
35.17017420820171	24.93247092185442	46.15652573136587	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.18696396568704	25.85579700919336	47.54557318726004	n
34.66881790335534	18.71091891792473	48.24856965246830	h
37.35563772964171	24.41266854729779	54.21739578527446	h
25.22300688135884	20.41708392437678	46.93179449919023	h
24.76583011540897	21.21444545460701	50.15050216637940	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.45354102541184	22.22182952468254	48.66166806242867	c
29.41144825396575	24.28793214575419	47.89473520416563	o
29.60141134837485	20.36779654489225	49.63536564154010	o
45.90146339209471	36.56531459043916	42.23346811491198	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.55966309334319	28.04814271944011	40.39704101620721	h
45.86808784470095	28.94193011770120	40.99952672249801	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.15926197337409	37.82066972582192	31.19440339703241	s
44.94395420080353	42.7839999644279	47.12005621887226	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.98699968238944	44.72706088187184	45.27888115100035	h
46.87770628623260	39.35912303928927	45.55359945141378	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.83231453927628	33.35079837486764	41.33376931648927	s
44.06769468651027	25.72610867268704	42.43239618195374	n
46.02228893508986	29.63307297943845	45.52547914571884	s
40.22119666949149	25.22744455384670	41.64405873077269	h
40.19894536366195	28.51233829917416	44.74550126742515	s
39.64722938640552	33.99041565915709	45.75010555319504	c
37.84613639867942	35.23309969577284	45.88106684574264	o
44.42571043139584	34.93879902101678	46.73167435182498	c

45.61320234571720	36.69318173490852	47.42392183682225	n
41.86753042980941	31.46446406517764	49.33716546576063	c
41.23641667364267	32.62915273016786	51.11777488616284	o
40.11477859530218	26.83256751360384	49.91547434313276	c
38.35096319952253	25.93912453669197	50.93985552439226	n
45.00744535748779	27.84512718199521	50.63364812550105	c
43.38761449766160	25.37223931480367	47.80407707145574	h

Table 8: Coordinates of $\mu - \text{H}$ in bohr.

39.96653877042216	39.94108136996629	29.65403824478054	h
50.18563956026507	38.72062182171678	52.89433384271663	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.75144262447033	37.19945934293511	31.46591649476167	h
37.16776367644133	20.82831243794387	48.70702279398838	h
32.51460957827533	20.98078795376490	50.90511403741347	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.36344532487447	44.92300839490792	49.80317471297406	h
48.20145170184552	27.13819263051758	42.48046460851656	h
46.78058234433258	43.02444385217571	46.49910347574785	c
47.25502908432220	40.94954859720536	44.87669828420985	o
36.36266415844197	30.49134966466789	40.21626874669367	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.29226336974215	27.95070603150701	42.51397077183415	c
41.88474333487050	26.78397325233627	41.89272701472814	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.58429692489555	19.09727997498647	41.85293349464716	s
42.38050261062239	32.12566188337702	45.50223041283330	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.12133995939346	28.02270248881138	48.15760371512805	fe
37.02916688627874	37.14043823289300	38.45022382873341	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.55908409688759	26.46873602387778	34.11898100595105	s
36.61354293836292	35.35175996549927	34.65032801542424	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
36.18554161369807	30.20840408796109	36.03713764540211	fe
33.96814701676301	33.98505121094873	38.90801148186114	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.34375145544639	21.13989935731260	51.42745876146917	o
42.80312670505579	37.78591634656405	42.53990177180473	h
40.55232108593291	21.97539034664317	56.13728232780117	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.66670757767368	24.57787679111288	43.38956298396234	h
47.53763572927446	39.43989189175245	49.56363801300957	h
50.64187974075264	43.39601304568947	47.85895799098043	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.76041353712547	24.68677907196615	57.13508739023964	h
39.27888926199616	33.43669558795221	38.71966634344561	fe
41.15329827682373	21.22042834499369	45.16059330859928	h
41.59065685906300	17.95225310626490	45.72702491149987	h
43.06731658599358	21.27019244810791	40.60425527809879	h

39.82478846506603	32.33543746689375	34.69565282199670	s
32.94363750267608	32.95093671329210	35.01289586064299	s
45.90464444280222	29.25843896705844	52.77546454604988	o
39.21081318567764	25.21161437842061	36.68380108922430	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.89574044923437	22.59950759502585	34.99206110620838	h
34.52453210351091	37.53408227331822	43.24490846505877	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.83645775115766	35.54927065723308	41.27206210880154	s
32.00476008480507	37.14131026632714	45.42876433946186	h
33.64184960629644	28.79508829356143	44.86760784919299	h
35.71427507378434	29.60415930253778	47.40092665760685	h
32.37941033600927	24.96389677676371	47.75939871629466	h
35.25143708106231	25.69443164678082	49.27948597359389	h
35.29606581183904	24.95933931272106	46.26638445663853	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.22512689944270	25.87264274594463	47.597197406660801	n
34.57772232209481	18.68965504467600	48.33498197613305	h
37.36833237102962	24.46986220517596	54.23557372249196	h
25.29354273812627	20.45516814760000	46.87760809625392	h
24.71744045594889	21.16024575380018	50.10505312223881	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.44907203452217	22.25775606912529	48.74895494439312	c
29.44733081580403	24.21069358240952	47.76911863519963	o
29.55794641339421	20.53746928441675	49.98368267448219	o
45.90422381703154	36.52847741239304	42.22989940734411	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.65603795618706	28.16577777465973	40.35457724716090	h
46.10768589581615	29.39443851851371	41.02635200696100	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.15770573476124	37.82468496234152	31.19306867606715	s
44.85715789754268	42.92530424432909	47.31924814644053	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.87972883135431	44.76030257944685	45.34732438862877	h
46.53216232237548	39.39807250332394	45.67486174248908	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.77091730412357	33.37928350366038	41.33912942673890	s
44.47620494262255	25.97532980914841	42.06790480795919	n
46.11758706131938	29.80381969611428	45.53826033043206	s
40.66813087868525	25.15167440589407	41.48028252032616	h
40.44638221164480	28.32305846292112	44.73317029561735	s
39.51758397748209	33.66326690283055	46.00480158470253	c
37.61494116070455	34.70080153102126	46.39355896374916	o
44.18838536441530	34.93762520464993	46.81402227492640	c

45.30483200807575	36.72439455770917	47.55717312601877	n
42.18283942258083	31.16555599994619	48.44871215778449	h
44.86199965421542	22.79796123810326	48.08437579548407	o
40.17633496723899	27.13196010182713	50.02022396572862	c
38.34570295206237	26.43944501700111	51.07721118715803	n
44.82367679841645	28.79065812024326	50.92527390666009	c
44.13572333022725	24.88241616000620	48.05418834848305	c

Table 9: Coordinates of **5** in bohr.

39.88027219052778	39.95638484457017	29.63462031514473	h
50.18591790742596	38.72099296038720	52.89659724568852	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.79886015194419	37.25401039524643	31.44824869364497	h
37.16932325472249	20.84065510452179	48.71957604094586	h
32.52159146393396	20.99665554953952	50.84618845043922	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.46300701504815	44.91771038205766	49.83287573225202	h
47.96127745462134	27.04953331921303	42.20815024092838	h
46.70021656135332	43.13069688650311	46.57561225109031	c
47.06600581208183	41.11002612020432	44.84376392193698	o
36.29152090884043	30.44226170841802	40.14531906752063	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.11774104288056	27.97240343487136	42.42246107562851	c
41.53089802028904	26.89472053058734	41.85395729727187	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.27873804344440	19.71221912412268	41.54593685381056	s
42.37221549670083	32.10034920598904	45.53724470053022	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.00313994338445	27.97778472599124	47.86587427696630	fe
37.16341841847144	36.88306343216814	38.49793216314217	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.38703766697773	26.31537368893769	34.12600605811428	s
36.52431283007441	35.09759351206613	34.52362148057197	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
34.12478783011036	34.06681169440390	39.00255249761528	fe
36.18544051593157	30.11962512744925	35.81958585288303	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.33428375495030	21.13508040500743	51.42089998648389	o
42.80332331097946	37.79149192400843	42.53391307886646	h
40.56049459822916	21.98825176438486	56.13898696797435	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.02801857282352	25.33403264323224	44.38231472430510	h
47.56867009200424	39.43434012536699	49.55724932456361	h
50.61325785478093	43.35198579260162	47.78405694192393	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.70109148295501	24.58607826839909	57.10680346179367	h
39.21351659606071	33.09346932638870	38.82710570394389	fe
41.08076935297919	21.06704986674231	45.43416656920771	h
41.79656545505078	17.75141340824964	45.39715860155135	h
41.51731169331262	20.45176304099078	39.84577299423113	h

39.75694603997304	32.09199533307262	34.63611983714317	s
33.00460015299183	32.96507139845028	34.95918009640052	s
46.48101434431327	27.16817911367397	52.05784093639915	o
39.16694654812960	25.31710799909564	36.64999939835042	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.96616435419872	22.60198999165990	35.02190360255885	h
34.52788393926121	37.55958926425264	43.28759718480084	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.90565529207788	35.48382179937969	41.28084105116928	s
31.97002863005782	37.14306068648829	45.41994982878668	h
33.71065685459562	28.93048351685893	44.87545082184230	h
35.73108422637328	29.49614334564203	47.53120331241702	h
32.10928729363503	24.99008466963175	47.63899223101158	h
35.11052059537702	25.46047059232177	49.08497644315852	h
35.01352847825954	24.89669333745949	46.04820253923394	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.06016896036906	25.82398475884837	47.45332285128870	n
34.57891687361903	18.68875699667020	48.33422458409427	h
37.27859961704729	24.25444758957508	54.19990798212408	h
25.24105195537209	20.42273540233027	46.92302501656936	h
24.78285922837365	21.20354867905846	50.15093583163834	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.44679603230346	22.28171665196397	48.64203103919753	c
29.36876388398004	24.30793598669001	47.70083925900863	o
29.64881687217525	20.55112213416455	49.75267930991216	o
45.90273791471996	36.51356428256886	42.22885888571659	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.58560173804027	28.19024268601153	40.22952658886248	h
45.74098149254182	29.26814092377309	40.83856622894535	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.20011585004301	37.71216917439460	31.25796595610304	s
44.80593019147150	43.03892478213246	47.46132965297539	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.79124464047878	44.89731714404968	45.47693347972255	h
46.47515237266622	39.52767921352780	45.65542964018069	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.72227510530318	33.40495939979093	41.31165404269372	s
44.13414712837736	25.95572334583989	42.44087360968657	n
46.10800013284381	29.75702016313552	45.37821859736875	s
40.35197029774125	25.25535186573843	41.38022238245529	h
40.18480145314942	28.46048313040566	44.60671571913852	s
39.55882047746860	33.85087323689648	45.80148145043939	c
37.73227937649820	35.03393717082353	45.99968976411265	o
44.28898659912767	34.89028268380505	46.75080857069632	c

45.43684258219919	36.65162130689886	47.47167900037656	n
41.93043643117277	31.23452502853679	49.23054107755314	c
41.32116573490397	32.25459024888885	51.09617486631017	o
40.27766662283800	26.52683616230891	49.64703285490692	c
38.51896775104967	25.63177141564384	50.66635303308325	n
45.10251123239360	27.55011147442076	50.39763854903288	c
43.60578711701084	25.16514823491901	47.29828305682668	h
44.57602845770754	24.40121403896081	41.33830496164635	h

Table 10: Coordinates of **6** in bohr.

39.85919543693208	39.96145550995704	29.64687438494431	h
50.18627868924815	38.72102082745959	52.89601491627009	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.79183702590741	37.26138759557200	31.45668099317638	h
37.16350463125293	20.81340210578796	48.68179432703638	h
32.54705215167962	21.04087394952680	50.87893936952838	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.44608722209637	44.91799726976721	49.82874786398121	h
48.23210635147092	27.29508448625932	42.12614757671192	h
46.71106354415723	43.11391948282038	46.56405930247919	c
47.08786813638773	41.08139321703991	44.84974158950288	o
36.43312347990086	30.58691826584312	40.25511168459810	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.33329156255505	28.12411203254968	42.21531791767723	c
41.91222476138296	27.02322422885318	41.46026738066848	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.46676197292395	19.67942989041548	41.74994735711783	s
42.38879331901013	31.96185691177643	45.57584808083732	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.12434208774537	27.68307011947095	47.81084057683411	fe
37.05998365641219	37.16862264012236	38.46673839594209	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.61713530299268	26.57294523890526	34.18872806457857	s
34.01242301191959	34.05386266972297	38.95229554532010	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
36.26240853132657	30.23999591015911	36.12246889692786	fe
36.63218457389787	35.38714073822548	34.67200879904734	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.37010501496005	21.17077580066201	51.42130885947473	o
42.80509173200783	37.78318508958942	42.54297406740572	h
40.56061953782881	21.98672823303727	56.13980581415392	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.42843900405121	25.08922105134780	46.61762703271295	h
47.57216056370913	39.43462109280253	49.55631737456896	h
50.61764360437877	43.35921508352060	47.79560650886024	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.70583149906831	24.59262911682585	57.11061537324892	h
39.35509303558577	33.54272533022711	38.73407491767546	fe
41.03260010020612	21.05826479753869	45.44502496653294	h
41.73595421447752	17.76129176590596	45.45040054680793	h
42.14062246144542	21.30115061766632	40.28388603644360	h

39.80919744187440	32.38963268977804	34.72637873604349	s
33.03589375113904	32.92311691208166	35.08411437553646	s
46.32224797423066	27.57243811005687	52.31929208980389	o
39.25726066551325	25.12896558509877	36.66030143653985	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.79978898555621	22.61729628699739	34.93476224644002	h
34.52755311635620	37.53762250122401	43.28083330265504	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.85919930853193	35.59159122575892	41.21698781963339	s
31.95819330658153	37.11545967076189	45.40729046895436	h
33.70186578352063	28.92559158446949	44.87587406891114	h
35.74062138667750	29.49154441075214	47.51242473644630	h
32.12584906867669	24.98031104233318	47.59643688883508	h
35.08796995574416	25.47154887074523	49.09561802013697	h
35.06201077336272	24.91474686621590	46.05529608277056	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.06646760139544	25.82454793430744	47.44381190174015	n
34.55262183511220	18.68320560776847	48.36186478747865	h
37.27612074865164	24.27147143560071	54.20284838282620	h
25.25802493741151	20.43295000253253	46.90841309980204	h
24.77188892763641	21.18972033513812	50.14026574035480	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.44461449164495	22.29580217531651	48.65821271344922	c
29.37229468652174	24.28076785422793	47.63857918497531	o
29.63746483018398	20.61505914520547	49.85224149259027	o
45.90695817801927	36.52827665866955	42.22030760574701	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.65773688655497	28.54796218384747	40.06957915713004	h
46.19540024414913	29.71940494748173	40.88865295541725	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.16600009392602	37.69065262283559	31.19622678185430	s
44.81204750263596	43.02662114969653	47.44056046208188	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.80575707984486	44.87332736246018	45.45384393497784	h
46.47988646803040	39.50303095349094	45.66099160059269	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.77760549274220	33.38636127272513	41.29515072440663	s
44.49965473423523	26.24692456475423	41.56188242226929	n
46.17275708510434	29.65999372955206	45.42580689221045	s
40.71948178303553	25.42544250371072	40.88527472879996	h
40.38342442526295	28.21281531063208	44.44303412030613	s
39.48577830555124	33.58781483841867	45.72054757145249	c
37.59187220368887	34.67090503945921	45.85684626256182	o
44.26693996597897	34.82543867996965	46.70807029319323	c

45.38236436760446	36.62003493152540	47.39530887998338	n
42.01571699453362	31.25405493964695	49.03211006353381	c
41.45515999930178	32.06086598865386	51.01948951866781	o
40.25913793817620	26.52138025355855	49.64044672745096	c
38.44866556923051	25.80057530211988	50.70469819038303	n
45.07161926631156	27.62339001778775	50.52159911003466	c
43.12843572202418	24.59865955929689	47.40860009407649	h
44.72481614206769	24.60239999423513	42.55187541252360	h

Table 11: Coordinates of **7** in bohr.

39.98164910649943	39.93790496783855	29.65811698391412	h
50.18865560334564	38.71955854951843	52.89145337639823	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.73965681473536	37.19002262166786	31.47188861804007	h
37.17097208529955	20.93744481138895	48.85092342180448	h
32.42559095119182	20.82364085258883	50.74715385208255	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.27452368252436	44.91702346720022	49.78287780291380	h
48.13305699336463	27.26925584954111	42.29016389651875	h
46.87858671577735	42.98142076306235	46.42114431814645	c
47.48303256124467	40.93109740555507	44.80840322589123	o
36.30615066293432	30.53164846577159	40.19603153445851	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.23147137899797	28.09209588276273	42.42043877222982	c
41.80095371993771	26.99803290800164	41.72271607607529	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.54534656308230	19.38714342660409	41.80447178423743	s
42.37648513421608	32.08226076016905	45.70594123095697	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.06380739894036	27.70891207039650	48.07668570878569	fe
37.00967536702561	37.15596767691576	38.42074915661474	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.55088971580251	26.46689990246218	34.12285805054863	s
36.60004780354437	35.36360626333369	34.62435499555238	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
36.14960647265919	30.22460651454029	36.02626884574574	fe
33.93869689669977	34.01826718477709	38.87940074675531	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.19998994882314	20.98225624866805	51.42717978334026	o
42.83159794821157	37.80467017225987	42.55077226654385	h
40.55488369603270	21.98237169103627	56.13687917015942	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.42240345185516	24.96948975606600	46.90897642105723	h
47.55366899606761	39.43648807696253	49.55260763509236	h
50.66762686231626	43.44464644064016	47.93989095168917	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.74508742995189	24.66254679084112	57.12746924706999	h
39.25587702990461	33.44770690997488	38.69575711287293	fe
41.08288106398198	21.14892767505845	45.30389374948017	h
41.65797786413858	17.84714812281264	45.59335139475949	h
42.63866638171015	21.37202118671032	40.46875683032690	h

39.80070084491042	32.32665957760065	34.68128975683164	s
32.91604484263237	32.97673685483809	34.98417239844350	s
46.24902689086601	27.63448676899957	52.58085755792394	o
39.21036850864029	25.21624020502000	36.67902916096447	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.89560462330110	22.60059502785114	34.99037268869265	h
34.52117992840570	37.53698142263100	43.22476876196585	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.82186680524582	35.54829345714666	41.28426391106816	s
32.02015613284564	37.14439958179491	45.43327452033535	h
33.67220026628891	28.86541611911293	44.87060158378507	h
35.72341254750641	29.56444450896374	47.44791561504810	h
32.32509419280015	24.97495902763218	47.72574070960834	h
35.28262890582498	25.58161231982470	49.14764319284052	h
35.17920487645485	24.95330574098370	46.11311965712455	h
32.35572687288521	29.36551238952182	47.94400165427532	h
33.97538600125975	28.60478435402797	46.90111269621590	c
34.18608675863739	25.84915598070994	47.51388180504861	n
34.69114150190082	18.71472215402243	48.22934067029608	h
37.35419806310379	24.40110895782209	54.21462657816237	h
25.18861415114565	20.40176148326891	46.95696773152188	h
24.79436345748844	21.24023023816724	50.17271527380407	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.45933284215756	22.20778671186942	48.61338059278923	c
29.41084436829909	24.28120101887770	47.86235288488903	o
29.61815705184928	20.33691649730068	49.54329311811841	o
45.91118755037100	36.49834417107112	42.20975281178318	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.57909522499703	28.47978092892987	40.28182191346611	h
46.03755090535935	29.65325680832233	41.06098742998381	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.14941150503920	37.84140794138643	31.17098532938995	s
44.92551519710157	42.81971689317976	47.15648257859101	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.97452604717873	44.72707160326001	45.28468611490205	h
46.76851829111338	39.36331023850209	45.57537765479755	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.72624913745857	33.39983789328969	41.31773394131976	s
44.39194297384986	26.17859862351359	41.83508886095321	n
46.13684491153946	29.66127017037903	45.61170536109734	s
40.58644105615178	25.40243497879357	41.18059958099121	h
40.31683512397867	28.28221382192852	44.67379361450177	s
39.51236502438173	33.74605752524089	45.82530131983681	c
37.62699000791838	34.85482583020655	45.96253678594010	o
44.30023249481921	34.92450106948176	46.77657198904194	c

45.46418253824592	36.71123400352199	47.42449193627220	n
41.98963620823795	31.30975788242023	49.14984788136890	c
41.40964557393567	32.14350294629377	51.13543693562513	o
40.20442607270805	26.53680608400341	49.87088072203557	c
38.37954223923196	25.78215141294300	50.90210529751154	n
44.99689646494728	27.66577772841753	50.76867674465541	c
43.09504907135414	24.50621510435375	47.57524567448959	h
44.58868011172996	24.65059593431172	43.00137351201103	h

Table 12: Coordinates of $\mu - \text{H}^{\text{Lys}}$ obtained by proton transfer from Lys358 in the $\text{H}_{\text{ox}}^{\text{cat}}$ state in bohr.

39.93948339496662	39.94469525276106	29.65061041272790	h
50.18753515644907	38.71727033734878	52.88759695985596	h
50.26532597612761	40.64384966141100	52.02713464999426	c
51.72791730508891	42.27462094631834	52.76220787699877	o
40.76504260777251	37.21759784001318	31.46086889431643	h
37.12600723542798	20.88614565726514	48.72349673648577	h
32.51057114082706	21.00180055153358	50.88466524676957	h
48.55707969954778	40.96887121655315	50.21873477851589	n
48.71770075099387	43.22511728239375	48.64276366150725	c
48.25362452735596	44.91461040066916	49.77548734767564	h
48.11883629840435	27.06996449970432	42.25156250577650	h
46.89744657326310	42.97694670077284	46.40366183132426	c
47.52329102961721	40.93870511356003	44.78121607832273	o
36.38470038016159	30.61638889065315	40.17960957462881	s
39.24105115677064	18.94452330032199	43.50905052240016	h
46.22803537449420	27.91916671974471	42.35616651613825	c
41.77269316856113	26.82346713506423	42.03053392256741	c
41.12452228829050	19.35004718838886	44.26890561780783	c
43.58488368074904	19.12359044693884	41.84647059717314	s
42.55304599921801	32.21990505763277	45.50429957402246	fe
36.36718023232001	23.76148999498827	37.77248262407600	h
43.38635698406541	28.16490409669979	48.14686651464378	fe
37.15428801217669	37.12182331256668	38.40864944514678	s
37.43969996373850	24.30660984163455	36.08670897057459	c
35.60617318643142	26.51904235761548	34.13320184342597	s
39.33084351899059	33.42593804791368	38.75027953237237	fe
36.89179466078398	18.18345311101594	50.71280934307384	h
34.05765876400448	34.08317975245841	38.87952126667342	fe
36.24837787941688	30.23211686040264	35.99935996554277	fe
35.78436412893236	19.64294339940612	49.74701000483825	c
34.32227708183861	21.03549231864609	51.49390567447793	o
42.85760202890791	37.80823433515327	42.57023008146829	h
40.55338925242471	21.97990219532421	56.13525312397146	h
38.98732518887225	22.68717502375104	57.35097313453696	c
38.83615087832501	22.33192163006125	59.63556509225246	o
44.60313654478329	24.59920825083274	43.40381053088377	h
47.55828189235109	39.42719492841660	49.54463861917236	h
50.67055110431050	43.45620295395945	47.95499079732714	h
37.24884518401865	24.02694171349225	56.12459001229536	n
35.76139593311585	24.69172366312235	57.13206695567821	h
36.71374609345237	35.32397209653939	34.57416688058890	fe
41.13403209069516	21.21166828775043	45.17400616278687	h
41.59655210561928	17.94235515278054	45.71362553405361	h

43.09319183437926	21.32629824742953	40.63927773783909	h
39.87872488194424	32.33085394342898	34.72408228619731	s
33.02735058248076	33.00484961397502	35.03187282321206	s
44.88577381559034	22.87068579114197	48.10641441820657	o
39.23122895517002	25.16627747874725	36.68095786698267	h
31.89727118913942	39.64356849057265	43.16713103624832	h
37.85058538612586	22.60746015160059	34.96334938466826	h
34.53142852678439	37.53631424100624	43.32971744811068	h
32.47179895374285	37.67779411713094	43.47525088092853	c
30.92573350235651	35.59421287177701	41.17171728725341	s
31.91655312583600	37.09753636164950	45.38987975075757	h
33.55113223358790	28.83555986760570	44.87543020772552	h
35.64294829141803	29.75465034926594	47.33328722096963	h
32.83470527126294	24.87906292858138	47.51202326960167	h
35.55611081244687	25.71109403707821	49.05317221253159	h
42.49004385572996	31.29088305708330	48.46209287230457	h
32.35447908672487	29.36437866723039	47.94215148011812	h
33.97407453132900	28.60368075397097	46.89930233858816	c
34.46006833934726	25.97313394949846	47.48350857240768	n
34.58944862558472	18.70136710639524	48.31303631043900	h
37.43442188881129	24.57159552920441	54.26569002556947	h
25.25787187652953	20.44855408604915	46.88531779895079	h
24.72334934817718	21.17359145426583	50.11550738563114	h
24.62496255328159	23.63589501726895	47.76380857707185	h
25.56800391979389	21.88976918051362	48.35626795287534	c
28.45011274163901	22.24893551367960	48.69469871797682	c
29.41573053509823	24.13488385250753	47.61453331057351	o
29.55266479220187	20.55809657673518	49.99526050781532	o
45.91305963914838	36.47403495778472	42.19956654907908	h
39.60187168362467	36.84896401816100	28.32450962379954	h
41.48006167297021	28.14649908404529	40.45169284127243	h
46.00164614565401	29.31727894624533	40.83284807300667	h
39.43517138323448	37.96880060202321	30.05871317843228	c
36.15334094836778	37.79221633285508	31.18101386753246	s
44.93950318631563	42.79935360403731	47.12334446617745	h
44.15765555110334	37.44255722963949	39.48606548723281	h
46.99173944116786	44.72739123956730	45.27486832169980	h
46.86997297730223	39.35831827958591	45.57948768173015	h
44.02135905433818	36.58935344310939	41.36828939951017	c
42.71584935922142	33.41274007889951	41.39482215675966	s
44.35862965895007	25.96888861886783	42.06205039311082	n
46.25233360385369	29.84009570561622	45.34439988411901	s
40.50496435869987	25.20066481665441	41.76263192304306	h
40.51986000614641	28.45806903773501	44.89664959976161	s
39.76425667196768	33.85545691389378	46.16730533045008	c
37.94885907328519	35.01593960633501	46.60353707955152	o

44.46124138996854	34.98922871797997	46.76448970598865	c
45.61662724383638	36.75207039520783	47.49990142172827	n
45.25339576598757	28.90722641625502	50.80722639406137	c
46.43512907907333	29.37150059023055	52.59432562796914	o
40.56442029624771	27.40338681469021	50.25326477984309	c
38.85107323142753	26.79548561262401	51.52093614248016	n
44.26011239074516	24.98384067181653	48.07583029603271	c

Table 13: Coordinates of $\mu - \text{H}^{\text{Lys}}$ obtained by proton transfer from Lys358 in the $\text{H}_{\text{red}}^{\text{cat}}$ state in bohr.

39.97848847285012	39.93366546430765	29.62233702944390	h
50.20146726426356	38.70847761376294	52.86715451793533	h
50.26435654662549	40.64306542506912	52.02613120542189	c
51.72691952969490	42.27380458463235	52.76118931461740	o
40.78549292836497	37.20678736193276	31.43478063058643	h
37.09692111142125	21.00147142165944	48.84544974532167	h
32.40409109218679	20.82461393841862	50.83637440654947	h
48.55614239538979	40.96808131103290	50.21776534901377	n
48.71676155710975	43.22428391317263	48.64182446762312	c
47.85643041192647	44.86024277569251	49.61752617987052	h
47.72478077243959	26.46213670508689	42.31870898778946	h
47.36849706190113	42.73680591802827	46.12105282279415	c
48.50956669887366	40.75928037922309	44.72594268706199	o
36.30389890917148	30.55535378947218	40.29861030336323	s
39.24029337659451	18.94415858317986	43.50821148400066	h
45.92911810960333	27.48165135659545	42.54295946436704	c
41.37973303551752	26.77858454628515	42.66664461120914	c
41.12372860331800	19.34967302261611	44.26805146159933	c
43.54050251862381	19.26258013935294	41.77411660088434	s
42.93842687237867	32.31185819973874	45.61736218343430	fe
36.36647914392764	23.76103079153990	37.77175318979175	h
43.60430123685996	28.36939163531935	48.48336182302478	fe
37.29505474835396	37.04916557364626	38.61943514394710	s
37.43897808835875	24.30614118955555	36.08601355136059	c
35.51387228213073	26.45978870187153	34.15798463419773	s
39.27944765389142	33.40755681902133	38.91711376841454	fe
36.89108223403486	18.18310162195669	50.71183046494110	h
34.14713250381133	33.96839024104522	39.08826156978326	fe
36.82072513007288	35.23447950576508	34.63650611447934	fe
35.78367437889674	19.64256356445499	49.74605002396675	c
34.19564314879060	20.84628724708873	51.52527539075699	o
42.70655033797810	37.71864779520583	42.50233988989922	h
40.54862647793521	21.97455177713059	56.13341493133890	h
38.98657307787450	22.68673660729004	57.34986575502771	c
38.83540065705339	22.33149077250475	59.63441424904233	o
44.10795217908052	24.59678394507041	44.23008988404171	h
47.63846811943269	39.38802004243279	49.47821526708203	h
50.72110480000521	43.68067838363915	48.31098306864106	h
37.24812708809115	24.02647873059162	56.12350719922574	n
35.79701387246877	24.75706195018389	57.13837391000521	h
36.11802398907720	30.27495239241157	35.91818844458921	fe
41.10155811220557	21.19144047269808	45.21004047689613	h
41.61536312403389	17.92296221624905	45.68746747206255	h

43.62599834799610	21.80850589914332	41.30733238368329	h
39.85326011650966	32.30085144513731	34.69021817205375	s
33.09655691157339	32.96483812051397	34.93700345356464	s
44.39149321710337	22.92955882812053	48.79397130576868	o
39.20056313265410	25.22246557119895	36.68577141816336	h
31.89665513842268	39.64280315149202	43.16629766702720	h
37.90156896988292	22.60174707439170	34.98745072557423	h
34.52909243839440	37.53691360351384	43.27970297238381	h
32.47117156466935	37.67706657257282	43.47441184252903	c
30.83977753054680	35.66801248159206	41.14618811444057	s
31.95222246093666	37.08701948497776	45.39649523906001	h
33.42734095067499	28.49675151526558	44.89270791084607	h
35.53355458764219	29.96548268293675	47.00963618521003	h
33.29870203528774	25.09052291732414	48.42281673713602	h
35.94870311767399	26.35107944822806	49.35848275798104	h
43.02282240517903	31.58296688901769	48.62993377988077	h
32.35385547710363	29.36381174939289	47.94122551431688	h
33.97341879636362	28.60312895394247	46.89839715977428	c
34.82658713330978	26.11142944095490	47.80256410546686	n
34.69002138416734	18.72755696285602	48.21573422150455	h
37.52158638775953	24.71802432976270	54.33183393505821	h
25.64908654265324	20.56512047389219	46.75178655472907	h
24.41871579912960	20.97886787549494	49.83987869435973	h
24.62448823202422	23.63543959327282	47.76288639072285	h
25.56751070127527	21.88934588186162	48.35533442816959	c
28.27425236879723	22.34671936696135	49.41348893329131	c
28.88487471243772	24.56099592577582	49.95637646436030	o
29.57728347713199	20.32491236337847	49.65096320143454	o
45.88550966476514	36.64640003023136	42.25955792122588	h
39.60110823427016	36.84825348113800	28.32396349294942	h
41.10390829604152	27.96620005684706	40.98335801420593	h
45.64027921020116	28.76438511398155	40.93107837342776	h
39.43440982360611	37.96806738828671	30.05813303251191	c
36.21102185264654	37.87253962348848	31.32310974378971	s
45.34611859827496	42.33527523925373	46.48018441280091	h
44.15680328462096	37.44183535425974	39.48530392760443	h
47.46456211006448	44.47406348854097	44.96864534619547	h
47.83705088385661	39.14081229853198	45.44398352515678	h
44.02051056730805	36.58864668553863	41.36749193508542	c
42.96081012539845	33.31829776646855	41.35162066817927	s
43.88574392484495	25.67040897632598	42.63411857019846	n
46.39384172412854	29.59340757861465	45.35021903129765	s
39.95176321418387	25.27211408400756	42.64624078731588	h
40.52911718874084	28.77449909604951	45.42658797946211	s
40.32538024847679	34.20703578190983	46.26196005517764	c
38.63822930471569	35.55480133547201	46.68730737554528	o

45.07511752941775	34.97904343045398	46.66806825541963	c
46.32705189312887	36.70098552098314	47.35743399492046	n
45.76753274128069	29.03280356434010	50.92586596411891	c
47.15798123599395	29.42183370340975	52.58441971785266	o
40.89769357938544	28.05408496869080	50.84716423516058	c
39.25370831645998	27.70191856306326	52.29329404298353	n
44.05918453380023	25.10443954594511	48.60357431477597	c

Table 14: Coordinates of **0** in the reduced state in bohr.

39.79814808759712	39.97133203832216	29.62507394507776	h
50.18872403792488	38.71797307564629	52.88746648346785	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.85403633938954	37.30898382822044	31.41921583294304	h
37.17086185601853	20.86200950209173	48.75209943564712	h
32.48409540163819	20.92008456536503	50.86659336539970	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.22682738249165	44.91400898400139	49.76721495656668	h
48.09213526320661	26.68521000489010	42.67699277120873	h
46.92721359345432	42.95461999513604	46.38443133802466	c
47.59179058736594	40.91302980955959	44.78123304700709	o
36.43441479812116	30.48092712763511	40.23620550063189	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.23824590444740	27.62032397030806	42.66385728491390	c
41.78131172084102	26.77262117652781	42.00068246778702	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.53830726226731	19.11308498094529	41.78105471808802	s
42.58854980910678	32.11259981190407	45.55722073434384	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.00888348081523	28.00699217109975	48.16238205245100	fe
37.22189391002399	37.12728288185006	38.45021022209144	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.63609621716537	26.60220756430201	34.19349819060651	s
36.81151342581588	35.17861808874404	34.77752749816641	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
34.23105460761463	33.99982960868655	38.88591870555285	fe
36.31385027134657	30.30656020835582	36.11115635745362	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.29756729803604	21.08870860695046	51.43099975687766	o
42.80002905975482	37.76956866639126	42.55287366959303	h
40.54832022634032	21.97043214015897	56.13566947656620	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.25155793198039	24.67443936268617	44.00888308246096	h
47.56015657203354	39.42750854379764	49.54882119802729	h
50.67751114878509	43.47076467110779	47.97914853819325	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.77836235875938	24.71396298459042	57.14298420804179	h
39.27694272506264	33.36951712887331	38.72363469511677	fe
41.15289085687890	21.23461247133509	45.13165630072140	h
41.58366904488020	17.97385980704065	45.74814354420419	h
43.83303272817356	21.63155511306837	41.31247066923011	h

39.95507283474272	32.20483545433888	34.74906066381950	s
33.09747971482373	32.95011320241835	35.04662071891324	s
45.13304335969715	22.97864071209167	48.98134778104848	o
39.25782814530833	25.10978123927932	36.68061776631595	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.79751015687541	22.61611187282066	34.93337510142074	h
34.53839966458359	37.56258318446845	43.38831781000044	h
32.47242634281635	37.67852166168906	43.47608991932802	c
31.02754741682462	35.58770789000878	41.10938558202930	s
31.86939394934352	37.09164264713268	45.37569364277695	h
33.62156124052045	28.75342454184159	44.86772392202192	h
35.70685134273737	29.62548212592075	47.37651676665892	h
32.40800179976306	24.98731942747524	47.86005610807002	h
35.31257699429258	25.77437146127382	49.32739442905730	h
35.29553355437127	24.94012540722965	46.33503389711732	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.24182982597934	25.89033639466017	47.65288165353473	n
34.61281518965971	18.69794427662832	48.29848390742529	h
37.38589757123381	24.50992925487486	54.24353395076324	h
25.27939927680650	20.44294005716090	46.89113305254981	h
24.72137260072651	21.17253118867680	50.11226193945539	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44856825417925	22.24378102413930	48.74249773720603	c
29.43344815709890	24.26164191876420	47.89230239466691	o
29.56605212901583	20.44620172445264	49.85213546917164	o
45.90446357898978	36.51711677225538	42.22365692245339	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.78517999021888	28.09494569413532	40.39748228704334	h
46.13479095800850	28.96290446224938	41.07948633527965	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.21475114362578	37.57775390579990	31.30021599939995	s
44.96168299468273	42.76497841958843	47.07857498688792	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.02217233123524	44.69878051672138	45.24642125801839	h
46.92951905932681	39.33428457459944	45.56456987924393	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.78845637696536	33.35093923133849	41.31999933811208	s
44.28196173560541	25.72771790269998	42.37532823097150	n
46.16635505347427	29.57956178108341	45.61742173950776	s
40.44024112007357	25.24345479618299	41.57926976246120	h
40.40704052178356	28.45913749239634	44.77313557056150	s
39.82036748737480	33.58530117563407	46.57677333220487	c
37.97134984256581	34.55509539489790	47.29100288005070	o
44.50806179728252	34.90282011970573	46.84304897129935	c

45.64428419637454	36.69989108306476	47.51850700823868	n
44.21508243831577	29.62453159367988	50.81804441152249	c
44.96049624667624	30.61246151456528	52.63751996781944	o
40.05828400651149	27.20236379461260	49.99647275059866	c
38.23351721706456	26.53795120687385	51.09455858676218	n
44.23228083577933	24.96994339575592	48.61129405234772	c

Table 15: Coordinates of $\text{TS}_{1,3}$ in bohr.

16.19061562191406	0.94109278952742	2.03180009695409	h
-3.89975998330333	16.17699512730738	-1.44258411653888	h
-2.06083326670726	17.05120102651253	-2.00269395274571	c
-1.78955363283380	19.33479898828629	-2.22790017396569	o
13.04940420744515	0.64826421691505	3.23026008794470	h
-10.23514343676046	-5.21533483724088	1.19500594518390	h
-11.40153031229022	-7.79848106835332	-3.04453129816191	h
-0.28201894744179	15.34838393308981	-2.48282233850120	n
2.31304556397953	16.21302623185450	-2.82700004737241	c
2.41543782646070	17.45392899931840	-4.49688109935969	h
-3.23120626889875	3.89505055878959	8.38294917299407	h
4.06835695194583	13.93573371533619	-3.15320238836022	c
4.16972014546582	12.36541592030822	-0.97778220540107	o
2.44576903793262	-3.22373072012571	-0.47793869126440	s
-7.39987270819940	-6.80481117952179	6.20487604716783	h
-2.34687502522118	3.15128347115891	6.66216910030221	c
-1.83811490853845	-0.89498077503752	4.41406152899953	c
-7.92154861253900	-4.93187527114877	6.91861804567341	c
-5.88606261185436	-4.18494823107820	9.63657348564197	s
-1.24846908773605	4.00237303575514	0.35002627509377	fe
0.30119399843210	-8.14529029601212	4.39664247158846	h
-5.89892957227324	2.85548239768686	1.70900378009340	fe
7.69057337166643	0.57643549203854	-2.55618282472457	s
1.87564010645789	-7.67442912717359	5.65714270929069	c
4.89154541255002	-8.45127424903812	4.11498747165690	s
4.99536828653915	0.04978889622741	0.73648221289805	fe
-13.37674951893450	-6.28667851166655	1.51413171929436	h
5.81586771682672	-3.22345859183764	-3.15208027061911	fe
5.57961073771011	-5.15425579384000	1.61324937108414	fe
-11.63641758247840	-6.57826136302694	0.42984655302167	c
-11.97356754576983	-6.19671022622641	-2.18989058330183	o
4.37998278116057	6.51537228843544	-1.02244948458241	h
-15.71302815040282	0.59009529669668	-0.62704592397535	h
-16.12002525033907	0.32146131112266	-2.67508874363643	c
-18.13515738043948	0.84549370394013	-3.69157998517498	o
-5.41928441130176	1.20676298125903	4.53388985297413	h
-0.59778623641886	13.48064391855665	-2.02980946762302	h
2.90554960075622	17.33970946262626	-1.17668171062075	h
-14.19043157328649	-0.59033532363900	-4.00431454105242	n
-14.49615351609244	-0.99353055836088	-5.85254988623347	h
9.75790544954314	-2.26343481814544	-0.10705494012673	fe
-7.73700734825103	-3.50948912405707	5.41988361796820	h
-9.87424325547020	-4.96125967955700	7.60165788274720	h
-3.74810615130666	-5.25385324886583	8.72491884558022	h

7.48581252890024	-1.72982402718616	3.61007900482589	s
8.31226695633896	-6.06682023659079	-1.57022780861173	s
-10.02547808342062	3.20116392773080	5.33108137777120	o
1.79303689444423	-5.65561833886572	6.12912696699872	h
5.95533582263630	-0.00673498390948	-9.85568897064832	h
1.71429553202181	-8.78859904689486	7.40298621924178	h
4.25115878877846	0.76217313910090	-7.04297616695315	h
4.47865847513931	-0.63907891930708	-8.54839344491288	c
5.23210292866939	-3.74851361555973	-7.22039755673458	s
2.68431001390544	-0.77281759776161	-9.58473589681233	h
-2.00673650654428	-4.40384205209929	-3.65569626154836	h
-3.92795408961789	-1.62777153103163	-3.84177949440583	h
-6.43060425791245	-6.82418616770777	-3.95077024825860	h
-7.54183099179805	-3.83458160728709	-2.85176441675788	h
-5.47633807354032	-5.37395795902452	-1.13956148464615	h
-4.05981390761735	-3.97782247050613	-6.30550396332374	h
-3.82859079841539	-3.64656103969926	-4.27418443923663	c
-5.94808796483970	-5.00944612839428	-2.98023762231323	n
-10.95081545793055	-8.51019598847365	0.83974618396586	h
-12.50461427184333	-1.11139555375237	-3.19186445141527	h
-8.05330426109950	-14.77326661556192	-5.93676472587736	h
-10.07411037754302	-13.36270644860183	-8.20663890043151	h
-6.69874652130428	-12.97636946537986	-8.46386977479416	h
-8.30084121226484	-13.10953657568203	-7.15810870667222	c
-8.50359357244463	-10.73838184704634	-5.47411669009121	c
-6.64967346583295	-9.19200243999978	-5.53599249651876	o
-10.48118500120465	-10.54745805566102	-4.16045419405004	o
3.61331109678333	7.86940723734079	1.94677363434553	h
15.39914953571164	-1.58753057171524	4.13719063353134	h
0.21552409081402	-0.67621085640897	4.66117435177370	h
-0.27462770111753	3.16963214203480	6.84489186381912	h
14.70981523983648	-0.40793328887624	2.58064779081375	c
13.94721608624006	-2.44700812099307	-0.12202118556787	s
3.48113856721580	12.85024419170179	-4.84444182211080	h
6.49943710690120	6.15121160467026	1.56805316454493	h
6.00208741686574	14.63002312528953	-3.49662409671221	h
2.60565229846698	11.32334881228968	-0.93757888487783	h
4.50304917023460	6.24406896700019	1.02466241730302	c
2.63832428850760	3.47347982582405	1.88730398677466	s
-3.30382485884478	0.60759938144744	6.19388767854240	n
-3.16157412932740	5.32650199618729	4.02471488063739	s
-2.35103758710609	-2.89382496589390	4.62197367188985	h
-2.64673519988599	0.07339093651604	1.13919112362584	s
-0.66805918138180	3.29936020943695	-2.82478684279543	c
-0.23623049649885	2.87917779055716	-4.94123419886317	o
-0.84039395987817	7.47094146005677	-0.50852972707526	c

-0.44517153252797	9.59603942877477	-1.04610693008144	n
-6.42405725249756	5.29796027261669	-0.56629098417417	c
-7.03819820170143	6.85653359974672	-1.98020152299046	o
-7.78623238366776	0.61848789854114	-0.31340356020627	c
-8.95120484338055	-0.79522977993133	-1.57661468731382	n
-8.39000389487536	3.06942603038581	3.85072049041770	c
-3.85516298196947	-0.38075308305065	7.77786791035049	h

Table 16: Coordinates of **TS**_{3,4} in bohr.

39.84829934403287	39.96361755706840	29.62978730966338	h
50.18591007743154	38.71873117052284	52.89006358194013	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.82994598081154	37.27570473164602	31.42885708155292	h
37.16955477031578	20.96337660770191	48.88998403171016	h
32.40345574685137	20.77898539271229	50.72198791993929	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.26327425921912	44.91752291937863	49.77748611616052	h
47.97106971388735	26.69155790676997	42.93361497791965	h
46.88974687908851	42.97604624939709	46.41094767665032	c
47.50827530420457	40.93074649875290	44.79789236024416	o
36.39856645036316	30.47958438330307	40.25304414506082	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.16530315750850	27.71204639084376	42.91593157138467	c
41.62883524103550	26.83672889352108	42.28803925172359	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.33495827995488	19.56182937966541	41.59305248130088	s
42.47041583478661	32.27898259174142	45.56264529141549	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.04151705945016	27.95958963993476	48.16636146638308	fe
37.16233291629239	37.18436657368471	38.49466415144827	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.63216628802412	26.57762282486271	34.17342573944013	s
36.77173470845845	35.25788104188769	34.79225656287650	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
39.22708126943234	33.42853767297574	38.75090224148494	fe
34.17820889092567	34.00324674455839	38.86693775577350	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.16636414577427	20.94167171325365	51.42721891417174	o
42.83144336862907	37.80646392915461	42.54825501401444	h
40.55514062406705	21.98613940816390	56.13574220014182	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
43.69849045191054	25.79458732682770	45.70770279603076	h
47.54380263062883	39.43144882584294	49.55262056817807	h
50.66958236369496	43.45113043629196	47.94799750100827	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.73104356478628	24.64494785489418	57.11660590757051	h
36.32252581000661	30.32320377789231	36.09898344659439	fe
41.10846132323695	21.10407254663674	45.37635056258422	h
41.75650087865858	17.78486519513826	45.46638742371021	h
41.78271104527856	20.85288709018763	40.01953744373679	h

39.99884020535678	32.32603146225736	34.78552463760287	s
33.06405306077715	32.97333569890255	35.02643625482227	s
46.21945678515969	23.72756747583476	49.68013471678533	o
39.25019372670472	25.13109016941171	36.68862675055837	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.82192294761217	22.60489287318266	34.95227347370523	h
34.53619729906014	37.55672871432844	43.35941653174974	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.98413242798326	35.56657610334231	41.15271978039193	s
31.90012015453701	37.10879799814437	45.39114699821454	h
33.66447960278835	28.85329804868771	44.86987097433039	h
35.71604640507511	29.57749511337067	47.43917035706474	h
32.34457446406109	24.98794287721837	47.80348371429187	h
35.36654761401817	25.59059065207613	49.12702749586219	h
35.12494085223050	24.93219402668007	46.10518660890285	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.19724467408184	25.85259709164615	47.53261315550949	n
34.71592602278061	18.72189221198038	48.20486871459076	h
37.35154610778761	24.37319462546068	54.20806703424927	h
25.18233241239653	20.39721197622397	46.96217763212741	h
24.79335315411705	21.24627833873744	50.17442356295138	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.45865799077050	22.19838657648126	48.61431491051044	c
29.41079674319019	24.29848568412529	47.94474775645554	o
29.61643159369035	20.29095008659575	49.46992275997652	o
45.90957018219376	36.50867402965380	42.21450252551195	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.71185502446448	28.05923629087219	40.60917123058727	h
46.01049873273807	28.90567972232135	41.21750760692863	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.20384383396193	37.64063984827612	31.28195555695823	s
44.93414212651449	42.80422279097819	47.13781136214458	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.98336816734313	44.72399684473255	45.27707111071062	h
46.82343493624294	39.35792130383727	45.58961498460253	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.72495091747607	33.39690362250300	41.41299158584707	s
44.10445723468685	25.87315935253779	43.04624470476119	n
46.10110212307683	29.87310720533634	45.67685006963633	s
40.35789724634256	25.23928287110416	41.91124311049585	h
40.26725201962095	28.70329970918223	44.92346462746862	s
39.75219079587917	33.97020196493465	46.30683970358658	c
37.96765581860741	35.15861042457336	46.82747587433468	o
44.39579987408755	35.01502757787551	46.84684158713676	c

45.56774938709323	36.78442755809098	47.54707382455297	n
43.31503517897659	30.33950514147714	50.54023348502563	c
43.57525962910880	31.64663299777555	52.29229607338117	o
40.22644747444499	26.55338132277916	49.80942058873624	c
38.42870099435765	25.67502380945140	50.79936159509150	n
44.93904307940139	25.44720181667234	49.10057469197847	c
44.5267982777226	24.13572509807189	42.28494026975803	h

Table 17: Coordinates of $\text{TS}_{4,\mu\text{-H}}$ in bohr.

39.97865174374265	39.93731532486163	29.65429460609664	h
50.18843010855773	38.71769197638795	52.88794213763953	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.74612056759177	37.19345977894047	31.46688644404880	h
37.17385869077192	20.85489858064904	48.74869094184101	h
32.49160240669912	20.93937281039560	50.84786205149346	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.23965527666119	44.91568615184489	49.76964539954728	h
47.97234642834242	26.55985751619524	42.84347925242682	h
46.90817696665798	42.94789419023849	46.39785290808341	c
47.54744071914269	40.88572448071459	44.81426450122440	o
36.32343326396328	30.50626642325350	40.16819917773834	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.14326963972891	27.53416293705264	42.73328908365374	c
41.70382110810864	26.72985974887630	41.86844798060197	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.54969168195408	19.09834777106111	41.79571164305204	s
42.48811294105116	32.19052953790662	45.42040636730196	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.74166737172849	28.01086698686054	48.03246963545078	fe
37.05728849898718	37.15442174784690	38.44741130514755	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.57118659991237	26.47715019536808	34.11374270628910	s
39.27915662972293	33.43611930038241	38.71225222459121	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.19027418152164	30.23484339694422	35.99825686977099	fe
33.97409522758412	34.01787191991041	38.87722017334694	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.30051355500881	21.10585343316099	51.42068016982409	o
42.76107594644562	37.75012607516815	42.53046782856814	h
40.55591105923971	21.98381800512867	56.13695202761792	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.02552963711350	24.67287869314555	44.07696292504043	h
47.56146798983145	39.42657267037944	49.54892916323872	h
50.67361176083042	43.46162641450727	47.96445948674216	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.73450793369262	24.63684723753866	57.12802365466696	h
36.64251584369682	35.38202187392091	34.63692894917126	fe
41.14777008144270	21.23956031651585	45.12326016613065	h
41.57210327100839	17.98047704505903	45.75839707095950	h
43.84803977518175	21.61853787133131	41.33099665800676	h

39.83990879991219	32.34729885288606	34.68897067100730	s
32.95922800615784	32.99196963523314	34.97844764113832	s
45.52422625005779	23.32544107982098	49.07924023595790	o
39.21501039191160	25.20006352876374	36.68271053138274	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.88800302442015	22.59807521762561	34.99142194191013	h
34.52555772483527	37.53705098345728	43.25043716874879	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.84244387907968	35.54826547152987	41.26608651867139	s
31.99683107274228	37.14283445325182	45.42720760165241	h
33.68981664584329	28.87350299048328	44.86834631599958	h
35.71708704178241	29.56089024826803	47.46725877653641	h
32.22590272840664	24.97100422249991	47.65311058598081	h
35.11474312343308	25.51511104362114	49.18453489217707	h
35.15074897218294	24.91818905910277	46.13806044143969	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.13050619510243	25.83589508410338	47.50471905395847	n
34.60795184086918	18.69603270570966	48.30411741219488	h
37.34315178191608	24.37632905345768	54.20878873205867	h
25.24636888080051	20.43112164573877	46.91051881228734	h
24.75971515724751	21.19400962254141	50.13779940807272	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44851305239830	22.25012654374587	48.67192316374722	c
29.40726741762135	24.25199192562899	47.73601485591571	o
29.59713823810964	20.49490592529306	49.80617589464384	o
45.89696996837704	36.56598028524004	42.24141546839957	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.78911266899381	27.98404331128409	40.21114313509258	h
46.12857652979363	28.84413260899615	41.11695332184325	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15388247880404	37.84221692200480	31.18131647469903	s
44.94693754186137	42.77924423995321	47.10998737703732	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.00614990792742	44.68238669683380	45.24455361139961	h
46.85314160106535	39.31489027409857	45.59923305087332	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.84743130163695	33.36173008941671	41.29462983368182	s
44.15648328607020	25.67668754694955	42.41447519225899	n
45.99573158201390	29.61175753374264	45.60463560477915	s
40.34140332147713	25.21282620770969	41.48665314492688	h
40.22640736825477	28.70086187179109	44.40759036526896	s
39.78136320475536	33.91008039465311	46.14562472769379	c
37.99959806595682	35.09669202300039	46.68042734415003	o
44.43084623626808	34.89380998819619	46.75368576484757	c

45.59410933682964	36.65839780158321	47.47810817036445	n
43.32175843137615	30.43238756618086	50.31298925868628	c
43.70897792219321	31.75413568553317	52.02859235790731	o
40.10176555820653	26.65054534419199	49.99707621704196	c
38.38944799013868	25.73910275376953	51.11688425578356	n
44.39628110549216	25.15945507207774	48.57105666940747	c
39.81867446083634	27.89900030317419	47.82747594831807	h

Table 18: Coordinates of **TS**_{5,6} in bohr.

16.10095443805776	1.74194416834125	1.93779851002017	h
-4.79506433053841	15.90239957499719	-1.44376471487185	h
-3.00966097461429	16.86572062789216	-2.03212643714248	c
-2.85968097097805	19.15843084904063	-2.27731084295590	o
12.98873287153120	1.32866364699541	3.18910261371462	h
-9.96700780097349	-5.80667293373634	1.44891960149358	h
-11.06766983305404	-8.37807438834525	-2.82942675352978	h
-1.14883065179798	15.25389195766176	-2.51545412922759	n
1.39456307818764	16.24952629195876	-2.89000162665357	c
1.44136440910818	17.41162640341482	-4.61853173533188	h
-2.75012877411212	3.62122335104529	8.56261291080269	h
3.28200847432663	14.06557972533398	-3.09341975146020	c
3.44625495679571	12.61136225502872	-0.84136731699797	o
2.49796990079717	-3.07514363229145	-0.33371400631165	s
-7.02682187386441	-7.16817527774006	6.40665911306852	h
-2.06880623149527	2.93256547686877	6.73049880749910	c
-1.56341227420555	-1.11925788170763	4.45198863164348	c
-7.63908935891009	-5.31916897128783	7.11076539806275	c
-5.57968203126161	-4.47043200725916	9.78846918746269	s
-1.64985357963970	3.85779009447741	0.37428304908790	fe
0.71750255349432	-8.12090527009520	4.53830957000086	h
-5.96065299210402	2.47953044712410	1.96358237322458	fe
7.59974471523895	0.90191198649846	-2.65394184342416	s
2.27624881687365	-7.55854545201061	5.78069300334277	c
5.32262608801385	-8.11842557974195	4.20846789694088	s
9.76182137723824	-1.74019864231430	-0.16361246133819	fe
-13.06337056644844	-6.99982146699051	1.76700920016263	h
5.83065311980534	-3.08656258219245	-3.26777930382446	fe
5.73462945306517	-4.75338133495706	1.70192056474633	fe
-11.31976184489160	-7.20929004904155	0.66909910852873	c
-11.67401783237095	-6.80288463783272	-1.94503307247723	o
3.99812621206712	6.63596608151151	-1.03767134939235	h
-15.77186009071311	-0.26904941751294	-0.40569849900908	h
-16.18366933650273	-0.57762124627004	-2.44745611407195	c
-18.23217591969665	-0.16740705796093	-3.44944181787505	o
-5.22864477832394	0.66967828912353	5.21531869048644	h
-1.36005061931017	13.38208893960537	-2.03234671207483	h
1.90437209526961	17.48731740597271	-1.29391011582982	h
-14.22089962759976	-1.39859008456001	-3.78726815724015	n
-14.52415774269333	-1.84906573723929	-5.62497807453927	h
5.07342276109646	0.34385799240759	0.80094355479936	fe
-7.54080669553598	-3.90451068291459	5.59702574429976	h
-9.57680347647777	-5.44506198699810	7.82373411996126	h
-3.47691581412866	-5.66461326848912	8.95389845793573	h

7.64586152051002	-1.30977695463860	3.65557758048064	s
8.48269576165630	-5.72058604669809	-1.50771382904443	s
-10.31150871255025	5.79062018469616	2.69192867137482	o
2.06466318071285	-5.55243713925271	6.27326290694182	h
5.81517294621940	0.18456010199750	-9.82718245205279	h
2.20098883784231	-8.69052614433796	7.52237868997753	h
4.22379020752183	0.81674329839448	-6.92588032641613	h
4.38492805933963	-0.51308709910151	-8.50160949523641	c
5.22122266526593	-3.68532280496426	-7.36270013790451	s
2.55227760566308	-0.60171459767828	-9.47390112202647	h
-1.84890883353916	-4.55740804134949	-3.51706341668864	h
-3.92931029174474	-1.89945458821324	-3.71525611644437	h
-6.13577834084855	-7.24429025312861	-3.75657144578042	h
-7.41160028138483	-4.32767043898513	-2.67169575766264	h
-5.23518489117978	-5.70310585571639	-0.96351921029249	h
-3.94809707855998	-4.27311674397600	-6.15509121240487	h
-3.71668688647164	-3.91376642404722	-4.12857348240137	c
-5.74719882388460	-5.38309601470515	-2.80202636826435	n
-10.56007498157359	-9.11929380851487	1.04929410577416	h
-12.51913066024695	-1.85270998136981	-2.97174503982327	h
-7.34234847147071	-15.23085431341207	-5.63908651995846	h
-9.47681195490357	-14.01535296548010	-7.92100286137097	h
-6.13349353252232	-13.41401113866712	-8.22014234782312	h
-7.71499587789883	-13.61971160682492	-6.89878348026547	c
-8.05366443188861	-11.22589658228551	-5.26417481933484	c
-6.24494840797021	-9.62331636545971	-5.28801100532194	o
-10.07815424110701	-11.07284564657132	-4.01880601028037	o
3.19127211930302	8.05093401041004	1.90598915480981	h
15.45052740959796	-0.78897766471995	4.09033865371438	h
0.48973140395624	-0.79194522985141	4.55331862934808	h
0.01105279611068	3.02863006733508	6.64336951585745	h
14.68709695236180	0.34046439703560	2.53117476086141	c
13.97082054240910	-1.78722603433444	-0.11892348923447	s
2.78020057712421	12.86688932408522	-4.73377966150850	h
6.13766226835406	6.45518350050610	1.54354719615601	h
5.17587121283051	14.85414571653162	-3.45218699960595	h
1.96595218035493	11.46166784210578	-0.78493781880374	h
4.13447131763747	6.43964239285416	1.01776680667292	c
2.49159418495344	3.57056343478909	1.98985621904742	s
-2.95521866567529	0.32635887556069	6.37058405307565	n
-3.31429090008347	5.06210082186077	4.27326126224346	s
-1.94242316217830	-3.13985467557002	4.72447062724584	h
-2.64509871415472	-0.27051499983994	1.26402529841329	s
-0.53044200117077	3.01534215384264	-2.63797934673569	c
0.21422458147923	2.51067305706446	-4.63168578199434	o
-1.27127322496409	7.35096072788465	-0.40059582332138	c

-0.98000862150050	9.49397690128955	-0.91441517375939	n
-5.07312383224761	4.22144433114262	-1.17001473705172	c
-5.97855705459584	5.03661575666943	-3.02108751964795	o
-7.89912200835029	0.19865569883351	0.01704549589767	c
-9.02667075407103	-1.27319583894737	-1.20620954167458	n
-8.55677880493589	4.51304695339863	2.38960984476169	c
-6.98720159053408	0.87874988607629	4.33107617605380	h
-3.19157137448411	-0.68000342271660	8.02059037294433	h

Table 19: Coordinates of $\text{TS}_{0',\mu} - \text{H}^{\text{Lys}}$ via proton transfer from Lys358 in the reduced state in bohr

16.01403581427251	1.68953252614534	2.08417405437158	h
-4.55749288486572	15.94156076905856	-2.02043029129957	h
-2.75074770850279	16.86542016143829	-2.60088297816018	c
-2.56378198514818	19.14938850953254	-2.89589379271130	o
12.85731848019724	1.07534713026818	3.12867216537320	h
-10.13696464780691	-5.45974433961813	1.03052319648046	h
-10.89683142926627	-7.97458727005941	-3.08600465788237	h
-0.90859165925367	15.21610310434026	-3.02488838772949	n
1.65345744703789	16.16565457735316	-3.39067133538775	c
1.72702303534492	17.37279762373936	-5.08675921144945	h
-1.96250531731389	4.88459920897660	8.11537374467216	h
3.41142042297291	13.86234975942569	-3.65905069315219	c
3.35736945991183	12.29000285980759	-1.50306937813419	o
2.68749146957915	-3.21265999492706	-0.42023475345862	s
-7.22482737724124	-6.90763306770882	6.32807674188678	h
-1.40539384354296	3.70653871124762	6.49661866955829	c
-1.30936037087250	-0.62217046877553	5.02880628028816	c
-7.81781398663361	-5.03445149493955	6.98268920994131	c
-6.23460074696022	-4.17229834763863	9.94068953928162	s
-1.40339565247886	3.42519698612058	-0.02447154329075	fe
0.52568779290297	-8.01556248725744	4.57663510554185	h
-6.17761456107079	2.79316608791704	2.35119776493633	fe
7.95624625746799	0.63699458176220	-2.91978277230081	s
2.07765371894583	-7.44793222301023	5.82489936658474	c
5.16550698225540	-8.16392847841448	4.38242258506354	s
5.83936239447325	-4.90643874403590	1.69973454158808	fe
-13.20225976745709	-6.75676489279383	1.61263180383353	h
6.03325127320465	-3.28362966966866	-3.25878069206045	fe
5.39097780645153	0.08948773136806	0.47912143633947	fe
-11.44912871595641	-7.01658522744532	0.54119110603241	c
-12.15966157149545	-6.99051904652057	-2.03989144636016	o
4.06590590297035	6.76580818964839	-1.26408180709863	h
-15.76190520694840	0.00124094043224	-0.75817714412956	h
-16.17615956488200	-0.38760739467581	-2.78332469717156	c
-18.20615628068161	0.02954964741652	-3.81922531573992	o
-3.96888663821505	0.97632273110323	7.25561638663151	h
-1.15637758443494	13.34109899129853	-2.55828625839542	h
2.21808565409029	17.32341233471152	-1.75211957601290	h
-14.21013952704405	-1.26737317161883	-4.08008877921241	n
-14.50309173448058	-1.90385574234608	-5.86271569186250	h
9.88044252260849	-2.01209152604926	-0.30644473813171	fe
-7.46035170640762	-3.60725918094564	5.52055625163212	h
-9.85036896822788	-5.05286239602083	7.38498432696967	h

-3.94231787041061	-3.62889356892626	8.94571993422058	h
7.87566545087860	-1.39469479215947	3.52406214485452	s
8.64446847336845	-6.01648607717794	-1.52380231627454	s
-9.20936505301969	2.05735414270197	6.91161314049581	o
1.90918556505906	-5.41598090298150	6.20287799346677	h
5.91650950967218	-0.11490479703024	-9.90846524186714	h
1.91307603301047	-8.48077883154732	7.62342735158245	h
4.29323113736956	0.59820411757028	-7.03748277963098	h
4.46046608173399	-0.76121002903929	-8.58513916941338	c
5.26581871143773	-3.91730599810462	-7.37199905307429	s
2.63292755761056	-0.84103747641812	-9.57140424286428	h
-5.09609651139604	-5.08012534396767	-3.16198331795855	h
-1.80629639671085	-4.39371241549575	-3.64044685722160	h
-6.02001020904589	-0.93363640205272	-3.02472740783343	h
-4.24593135908255	-0.23722437238001	-5.49136468107130	h
-2.66711422114569	1.14461725421663	-2.27338734104403	h
-3.95440309463909	-4.34457106821426	-6.25652037243778	h
-3.74179756722056	-3.94264332896325	-4.23607244274776	c
-4.25549065414572	-1.17582856798098	-3.80608930345617	n
-10.57646033084809	-8.83192649900597	1.12071331872032	h
-12.51461922902523	-1.64014481473902	-3.18531685953308	h
-7.11673553231159	-14.28118094765966	-4.99581924425863	h
-9.12832417181030	-15.10137958929267	-7.61238879804003	h
-6.25070379542505	-13.49666397992209	-8.14113478826326	h
-7.85060073490224	-13.64912141450820	-6.83497876738119	c
-9.31579095700733	-11.10620583691241	-6.58045185161353	c
-10.67171461744474	-10.48286152231728	-8.42306633661577	o
-8.96368647132586	-9.96399428521005	-4.49197235827187	o
3.16395781021514	7.89251539656171	1.77726129597829	h
15.36958666021224	-0.91207631422816	4.14343239892219	h
0.74090927267259	-0.51792734764506	4.70244304641736	h
0.64338149822933	3.86004535564211	6.17291157232634	h
14.64167927467371	0.19256120241072	2.55004367621948	c
14.18014636798525	-1.91265668336690	-0.17177347289447	s
2.88366629743700	12.80934473388789	-5.38954046235518	h
6.19699966867885	6.40706918363764	1.32024581887002	h
5.36957676495974	14.54110044850912	-3.91416255453779	h
1.95026480474659	11.02129435721612	-1.65850506079964	h
4.20030559638000	6.40882284948164	0.77052826856164	c
2.70789723435242	3.36025586946707	1.51099326756559	s
-2.04656646502563	1.10918502988330	7.01375159356834	n
-2.90867587339831	5.30371556153810	3.69410399715809	s
-1.78613939068015	-2.56690918075741	5.59138530285681	h
-2.85413614840858	-0.19575220443238	1.89269778040224	s
-0.42364047242518	2.62860831909120	-3.04399676277837	c
0.38962594964001	2.40678875627188	-5.10618693732465	o

-1.23936439059535	6.84108261616551	-1.24365536899917	c
-0.85731254492556	8.95378448853528	-1.87932422655559	n
-7.81310929143264	5.42357529740564	1.14992260164600	c
-8.99839988588159	7.13586829198990	0.41029582286621	o
-8.23743429762547	0.68126433632088	0.29417574924185	c
-9.53470461306418	-0.59345725541171	-0.99268227612074	n
-7.91881523688616	2.25181268183553	5.10926841950611	c

Table 20: Coordinates of $\text{TS}_{0',\mu} - \text{H}^{\text{Lys}}$ via proton transfer from Lys358 in the oxidized state in bohr.

16.03311642743863	1.64564045699205	2.02575660942049	h
-4.55867422168084	15.94285083118249	-2.02057585961010	h
-2.75080062083429	16.86574519433179	-2.60093400076555	c
-2.56383111802743	19.14975889585304	-2.89595048449505	o
12.88141710577389	1.12036328506177	3.12786443240203	h
-10.09429449346008	-5.53945226883714	1.14810355365972	h
-10.82150455886675	-7.87585381773212	-3.04860657665515	h
-0.90860866678879	15.21639601188963	-3.02494696923936	n
1.65348957238202	16.16596638216378	-3.39073747580212	c
1.70632819426537	17.42064534693749	-5.05046769391378	h
-1.98413130805013	4.89135513979166	8.20776002259333	h
3.41086640629254	13.88131713456351	-3.75504505647195	c
3.40252522764759	12.22896329845099	-1.64570604705357	o
2.66509201327328	-3.19126884119811	-0.38705108785372	s
-7.22496721697449	-6.90776723826369	6.32819957408491	h
-1.35235979621748	3.74158167580505	6.59904943854805	c
-1.06756620706329	-0.59838965053413	5.15939984696645	c
-7.81796516472360	-5.03454787097192	6.98282338049619	c
-5.92400637414576	-4.05375138475598	9.71308920147686	s
-1.38286400341645	3.37461249696073	0.07932182527055	fe
0.52569724153359	-8.01571744479969	4.57672392266972	h
-6.12182025357085	2.61033161040280	2.51975971793196	fe
7.80409593287356	0.57284429804797	-2.69975607418739	s
2.07769340319445	-7.44807584219573	5.82501086042612	c
5.14889902406866	-8.17320797716400	4.35927610989386	s
5.21484876545612	0.14428769422912	0.69510150948637	fe
-13.20251488048396	-6.75689528389645	1.61266203945153	h
5.93284520213521	-3.32104038836350	-3.28257428141528	fe
5.82870113115198	-4.95062524502550	1.73323208814597	fe
-11.44934981391304	-7.01672128772632	0.54120244438916	c
-12.06038384253510	-6.82486392905631	-2.05849427328980	o
4.05766647638812	6.70538137117292	-1.27201585678437	h
-15.76763644943512	-0.00273245916672	-0.75550862725289	h
-16.17647136969262	-0.38761495358031	-2.78337760950306	c
-18.20650776974086	0.02954964741652	-3.81929901505879	o
-3.66351050369122	0.82336426596482	7.58979438014846	h
-1.15890789151744	13.35337029811801	-2.54105680810223	h
2.24222023273866	17.27647484993311	-1.72839227280506	h
-14.21041353733217	-1.26739773805845	-4.08016814770966	n
-14.52971007682115	-1.93236260480063	-5.84928265920838	h
9.90684450101358	-2.09371666024930	-0.14294264042830	fe
-7.66373227841216	-3.65780431050580	5.43921628666852	h
-9.78607538783750	-5.10757011069715	7.62244195391993	h

-3.62944277191298	-4.41566447766548	8.64644735271054	h
7.75009469316969	-1.48721949526548	3.59739430224386	s
8.52643437096360	-6.01079514570020	-1.51221091777475	s
-8.94389861421309	1.66049131136545	7.15449677450487	o
1.92642341328546	-5.41814356606350	6.21470050972558	h
5.91662289323968	-0.11490668675636	-9.90865610420576	h
1.93430333104335	-8.49334316525971	7.61498664797351	h
4.28479529976426	0.60341988236303	-7.04312347221507	h
4.46055300913574	-0.76122514684829	-8.58530546531238	c
5.22066734850212	-3.91023456857967	-7.34637691960056	s
2.63770820025347	-0.84846780873359	-9.57549969994522	h
-5.03245872646154	-5.15405406994651	-3.16294884350803	h
-1.78268342150139	-4.33328793958776	-3.66881367366071	h
-6.11122210174976	-1.05612461870334	-2.93138991957920	h
-4.41660890119783	-0.24283003449698	-5.41661795132138	h
-2.76388038634135	1.20691416903503	-2.13400182692615	h
-3.95447868368409	-4.34465421616376	-6.25664131490978	h
-3.74186937681331	-3.94271891800825	-4.23615370097113	c
-4.35611205055110	-1.21434788130041	-3.75151503647555	n
-10.65209937560962	-8.88953562616364	1.02986265662829	h
-12.57571017345477	-1.79200331035936	-3.16575919416178	h
-7.16850030612882	-14.44104363848503	-5.04020547483655	h
-9.22727923130860	-14.94997657569583	-7.69860425194590	h
-6.25082473789705	-13.49692476212734	-8.14129163553163	h
-7.85075191299224	-13.64938408643957	-6.83511104820994	c
-9.10960041172447	-11.03702915457052	-6.42233013587018	c
-10.28810922675339	-10.12185838129998	-8.27142261809197	o
-8.83468787557331	-10.06739456713885	-4.24013846560090	o
3.16953161231728	7.92365997517176	1.73418737577102	h
15.36988334721386	-0.91209332176328	4.14351176741944	h
0.96533965550902	-0.42391343148394	4.75904112497469	h
0.67577448638848	4.04397818284366	6.25956303510991	h
14.64196273359246	0.19256498186297	2.55009280909872	c
14.13481950329552	-1.97318109350198	-0.12267847803920	s
2.86700593086652	12.87896569243745	-5.50948943615045	h
6.19711872142473	6.40719201583577	1.32027038530965	h
5.36313718207176	14.56910894375827	-4.00603914531505	h
1.96530614093878	11.01300729636766	-1.78400596361020	h
4.20038685460338	6.40894568167976	0.77054338637064	c
2.65333586252959	3.41526348738037	1.59901821989326	s
-1.80600895668440	1.12431215820558	7.13033442006682	n
-2.97998634082860	5.24887729089900	3.79472176356462	s
-1.45687661676894	-2.54563698599061	5.76278413484608	h
-2.72958605385879	-0.28076095269116	2.05944859375033	s
-0.45015678176396	2.52678380995657	-2.94661802304708	c
0.35237825366505	2.23325032807913	-4.99789358567190	o

-1.24569985857010	6.77301661601737	-1.18740483745271	c
-0.88580750039420	8.87196300775787	-1.85699882054821	n
-7.98443320949954	5.18170133589048	1.50428531838873	c
-9.28108925385424	6.84412359951073	0.87922055891245	o
-8.18524223371807	0.46662836447158	0.50016252264610	c
-9.49743855990422	-0.79432834400569	-0.77874009576449	n
-7.75615146987158	1.96370718019429	5.31075861116982	c

Table 21: Coordinates of 3_{small} in bohr.

41.12531597326299	19.35041757470936	44.26976355346858	c
43.34956314474169	18.63586448262361	41.70256780702720	s
43.74978092292350	25.04006316133915	41.06240666356563	n
45.66743058694529	26.77764875459742	39.90488964860472	c
47.50808652315001	28.47267841205775	42.30961237324458	s
46.33793054194805	26.84273748673231	46.22850276216219	fe
45.26001156273247	26.68574887134265	49.33697721721605	c
44.58758760439852	26.56659376292939	51.44515786958906	o
41.48277105643637	26.37527705856738	42.11263244461456	c
42.23486756801973	27.98654047895376	45.08848084433622	s
44.93015327962554	31.20645481017468	44.46743938112877	fe
43.38917011184613	33.20618950576494	41.01227784386234	s
44.02220943109442	36.59006775958463	41.36909064338717	c
43.60820630648914	33.02906210877461	46.84030965729769	c
42.80831400890921	34.33684879071617	48.44563322885838	o
47.85358662245226	33.27960243424840	44.78610190422864	c
49.63526319348481	34.60607692857953	44.97006232203544	n
46.81272863158732	23.35477868496029	45.56965651013606	c
47.22613370544878	21.19361666371659	45.12468152897230	n
49.37273338285404	27.56448910848844	47.32909472610575	c
51.38358205552266	27.96453617873794	48.15114548907049	o
34.28768647246135	33.89267115122950	38.95174723332414	fe
36.50126608106009	30.33563747836124	40.30496400052630	s
36.29477262345927	30.17490119276738	36.11695757755094	fe
31.02614345579070	35.56795275919538	41.12772042879627	s
32.47243201199473	37.67853300004582	43.47610125768477	c
40.05646000539456	31.97792798050649	34.72629688047538	s
39.61799739537366	33.05192500594758	38.81233122300017	fe
36.24475229718524	37.54073522593516	31.36348785259398	s
39.43593672231510	37.96953192603358	30.05928954490041	c
36.93691999635809	35.05421923947436	34.81779521116151	fe
33.12156776391864	32.93229037022299	35.10184577069943	s
37.46677752420382	36.86382859949706	38.58446597745868	s
35.53417179894354	26.45077766312297	34.12699167191037	s
37.44042372884437	24.30707660398742	36.08740061033634	c
41.26346096632716	21.33578199421176	44.85164506640367	h
41.49926669369655	18.14360943632683	45.91383158064704	h
43.22146772052038	23.58624346130973	39.86723574305868	h
46.93899709470926	25.59865914692253	38.76496839859557	h
44.66471170334651	28.14620976564074	38.70219165336028	h
40.01996686465964	24.93955948473345	42.43062997176158	h
40.79202652546395	27.74967026538254	40.71431639792926	h
45.82282359799313	36.75633082372434	42.38179652124317	h
42.49044956625506	37.48924736508459	42.43652288949177	h

34.53922336466172	37.58125223568286	43.34535813005810	h
31.90361781216613	37.11008177254464	45.39569667849288	h
40.88564955005324	37.32709889392359	31.39725143942048	h
39.77811112880310	39.97442251405803	29.61227734199028	h
39.19964041794422	25.23435481643513	36.69146761975011	h
37.92606096824210	22.59693320945883	35.00564244538410	h
39.24175035543688	18.94423984140324	43.51028262383366	h
44.15825081483271	37.44411058451423	39.48715019002856	h
36.36753172137927	23.76215517858427	37.77309300561436	h
31.89704820145667	39.64424501252540	43.16860502262581	h
39.60194916239578	36.84886764212862	28.32546582521879	h
44.67285746497734	24.19090131034421	42.62138692848207	h
45.45596354500896	19.57466296098344	43.11602894928819	h

Table 22: Coordinates of $3'_{\text{small}}$ in bohr.

41.12531597326299	19.35041757470936	44.26976355346858	c
43.29768894783317	18.73337091398500	41.63704535251938	s
43.49302043220089	25.24717611299856	40.14205309821934	n
45.40712281080918	27.10449595096811	39.19252155704799	c
47.28194992986964	28.39129779022441	41.82182482456325	s
45.92728980402963	26.12374405891505	45.32612258610754	fe
44.41388209407840	24.16991363055826	47.93433605780479	c
48.90084807278107	21.69739591866257	43.96893948509450	o
41.20187557931285	26.46365499394234	41.28226428392276	c
41.90485453197520	27.68186684218725	44.43300296628366	s
44.71766977374785	30.89527088041909	44.28002999851598	fe
43.25684144855003	33.22224290503019	40.99030324598215	s
44.02220943109442	36.59006775958463	41.36909064338717	c
43.29214937443769	32.49375193585976	46.76091550560064	c
42.40839743869527	33.64722030418253	48.43201420919132	o
47.59861854954722	33.01041610037147	44.77931221969787	c
49.32924970817977	34.38719368904113	45.04533272953358	n
47.62445988126026	23.47168159717134	44.48624646335436	c
43.51079221751577	22.81327139389353	49.45411464946871	n
47.80964862962018	27.77774003055147	47.52789180877249	c
49.17098331428429	28.53589613441454	49.09498226960113	o
36.16757948756893	30.20726638638564	36.11694012875248	fe
36.32134800122373	30.46140994797418	40.29275564842697	s
34.15696251027239	33.98385498539199	38.87136117235045	fe
30.94565079867666	35.61235994476638	41.13442205613885	s
32.47243201199473	37.67853300004582	43.47610125768477	c
39.94827872674936	31.98018984137591	34.73426238440338	s
36.84497863165776	35.08113939379665	34.75102804383423	fe
36.21416098751795	37.57538201405350	31.29991557504308	s
39.43593672231510	37.96953192603358	30.05928954490041	c
39.48397114731864	33.13631561205998	38.79139877302536	fe
33.02077856300478	32.97603418850671	35.02254794457993	s
37.35265456110591	36.94255207407836	38.49540648539703	s
35.50548510273990	26.44595689647582	34.14351072515612	s
37.44042372884437	24.30707660398742	36.08740061033634	c
41.27117806103482	21.32123263998937	44.90028254673680	h
41.53851474426127	18.11395200387363	45.87730488085673	h
42.98474090269443	23.93867972862488	38.79411872558598	h
46.66250930028660	26.09012352290007	37.88735945598874	h
44.41139736876606	28.63918669715303	38.20395818146267	h
39.73939364488862	25.00029241809621	41.43046812788998	h
40.54171986078770	27.96878932441100	40.01340493653647	h
45.84011304108001	36.68128092654315	42.36119865383848	h
42.53733976727089	37.53675662492057	42.46181479480905	h

34.53448754320699	37.56031248942626	43.30628838523307	h
31.92595484420336	37.10667739598924	45.40015675843663	h
40.85518394438478	37.30211870448475	31.41721173749650	h
39.81105386215761	39.97039592660052	29.62240301846761	h
39.19827686639276	25.24809195788849	36.66179333463877	h
37.91388308036566	22.59868482417764	34.99748833192974	h
39.24175035543688	18.94423984140324	43.51028262383366	h
44.15825081483271	37.44411058451423	39.48715019002856	h
36.36753172137927	23.76215517858427	37.77309300561436	h
31.89704820145667	39.64424501252540	43.16860502262581	h
39.60194916239578	36.84886764212862	28.32546582521879	h
44.40061387832566	24.29546222656295	41.70895491156208	h
45.43575593350025	19.57086073207255	42.77959285080937	h

Table 23: Coordinates of **TS(4, μ -H)** small model in bohr.

40.00777266276871	39.93011325433316	29.65346234472162	h
44.15765555110334	37.44255722963949	39.48606548723281	h
45.09215662731935	34.46803049443029	46.62721911092351	c
46.59169668808880	35.96703850616471	47.30546432190977	n
40.73776360745349	37.17708746729737	31.46592672933570	h
41.05918264394354	27.92470055382992	40.58318441633605	h
45.50644838231421	28.27492763255322	40.88729476943187	h
44.02135905433818	36.58935344310939	41.36828939951017	c
42.84936590883232	33.32520751240989	41.33788116990382	s
43.38928351456539	25.38048014369063	42.55930220551883	n
47.29962480339879	25.86371530867237	42.49153217317178	h
45.94443421886963	29.17986022661134	45.33346677753069	s
39.47463511619505	25.31541043113491	42.00722529582029	h
36.26943345393182	30.55805436064695	40.16395206911025	s
39.24105115677064	18.94452330032199	43.50905052240016	h
45.58061005617250	27.02893350652740	42.55192689058860	c
41.00133299695411	26.69765033248168	42.25920677832512	c
41.12452228829050	19.35004718838886	44.26890561780783	c
43.48376956707422	19.30843480072328	41.71922211232723	s
42.67372797111903	32.05516861150195	45.47324757315388	fe
36.36718023232001	23.76148999498827	37.77248262407600	h
42.92022209987462	27.89574206416584	48.19444045896628	fe
37.08498134016452	37.16893181103621	38.45875284487046	s
37.43969996373850	24.30660984163455	36.08670897057459	c
35.57231136620949	26.47997888063014	34.11247603715961	s
36.19514837749875	30.25836448495313	36.00561845022884	fe
39.43517138323448	37.96880060202321	30.05871317843228	c
39.27173559653450	33.41452580252428	38.75595173027635	fe
36.68430930185077	35.39820800959526	34.64967937116717	fe
36.15399004029403	37.87441985600240	31.18091536845005	s
38.76609129060825	35.56697066383303	47.06874393310425	o
42.72855117624793	37.73053002823692	42.51806192733662	h
43.93072002773799	30.38973891794072	50.24836897372347	c
44.58654975554805	31.67633074822655	51.91215155394825	o
40.82707299380038	26.77241149150789	50.95094814732061	c
43.34474185539853	24.55065720678002	44.32571168020578	h
40.02191524023542	28.74887025814083	44.95444943855691	s
40.29681884030833	34.11075851415463	46.41869491266669	c
39.78275902946310	25.99031887817178	52.76901298076071	n
44.46173904993292	24.97520340512963	48.57339226535918	c
33.96519422537174	34.06219638897213	38.85292642165486	fe
41.11140361405634	21.18831668042107	45.22629321104683	h
41.63297856982859	17.90606543982219	45.66735491831591	h
43.55767101790503	21.91898247784649	41.40578282345886	h

39.86862861707992	32.35482508373001	34.70867585016770	s
32.97292046282379	33.03605192569087	34.94085738558297	s
45.59320492900625	23.10028773365957	48.94746640199869	o
39.21075453141466	25.19831401960812	36.69474818333353	h
31.89727118913942	39.64356849057265	43.16713103624832	h
37.89472880070595	22.59744988413983	34.99259114837498	h
34.52332705806408	37.52808636022821	43.24001275163053	h
32.47179895374285	37.67779411713094	43.47525088092853	c
30.81310295539906	35.60441112101923	41.22808185803899	s
31.99358669381339	37.12824447904647	45.42217701677011	h
39.60187168362467	36.84896401816100	28.32450962379954	h
40.00199497254255	27.59667951350749	48.88137986782244	h
45.86911245428620	36.57024746616707	42.30270817007401	h

Table 24: Coordinates of 4 small model in bohr.

39.92758127160238	39.94453061658034	29.61366374536709	h
44.15765555110334	37.44255722963949	39.48606548723281	h
46.36003181363717	33.51919193626373	45.87025641095914	c
47.92457233133069	34.96266429090532	46.51416812937025	n
40.81795319444724	37.24085470466764	31.42181180393002	h
41.06837256108953	27.88885770182212	39.61467782773647	h
45.40375593742367	28.77923079135190	38.95613834552579	h
44.02135905433818	36.58935344310939	41.36828939951017	c
43.23969368422693	33.22154292211216	40.97397919681538	s
44.02085408264659	25.34099478493613	40.33386692354458	n
47.72076374353628	26.34291296647957	39.40746131952148	h
47.05278718873060	28.67102837528114	43.23658738917183	s
40.13562635985237	24.90573455322940	40.86225643929356	h
36.30806546848962	30.50390123448542	40.32890222390711	s
39.24105115677064	18.94452330032199	43.50905052240016	h
46.00283855410937	27.21217473367639	40.18846145832970	c
41.57954348330889	26.39325317134401	40.96814007915410	c
41.12452228829050	19.35004718838886	44.26890561780783	c
43.54371238873328	18.56206836320264	41.91331251760654	s
43.80687201720789	31.17685479979282	44.81645853959087	fe
36.36718023232001	23.76148999498827	37.77248262407600	h
44.81982744108481	26.80481146843961	46.43320062919054	fe
37.39864546989411	36.96419969720388	38.63778693062935	s
37.43969996373850	24.30660984163455	36.08670897057459	c
35.43532707636775	26.41196259281327	34.18361184538802	s
34.20713106619388	33.95136025022672	39.12096564636888	fe
39.43517138323448	37.96880060202321	30.05871317843228	c
39.33896073763066	33.28375031710434	38.89128453071348	fe
36.85597109180704	35.16646468728587	34.65151871950020	fe
36.22944863912459	37.81150484092542	31.36243515568089	s
39.88630709612731	34.39606352772334	46.94816585074557	o
42.52644454794605	37.53168231175951	42.44943179950754	h
44.18641723260276	29.66121290033736	48.48789978309755	c
44.03122636225957	30.50546986619002	50.53475292820384	o
42.84342765157364	24.78290080033452	48.68055846402277	c
44.51598384208010	24.10836747549896	41.76154629484616	h
41.20322016209845	27.74958530980234	44.18513410004003	s
41.41818548221539	33.05257468881891	46.11862803641192	c
41.70105790392315	23.40430682789142	49.99771562321916	n
47.59466126023275	26.10570219802261	48.05932074228644	c
36.06630914725282	30.21515633410139	35.94621271108146	fe
41.29498743107568	21.32057340602527	44.89381350035941	h
41.49102263412163	18.14730975732968	45.91565402651899	h
43.11094267063226	20.51960008211030	40.31614031837968	h

39.80911770320962	32.16600647261883	34.65687770197592	s
33.08839566788488	32.95787946894563	34.98702557554729	s
49.43467010235702	25.54369838407383	49.14153249573381	o
39.20061889763285	25.24314730204721	36.63479917983825	h
31.89727118913942	39.64356849057265	43.16713103624832	h
37.89903494566136	22.59966791610414	34.98971482374124	h
34.52992212843011	37.55246196572875	43.26239760224664	h
32.47179895374285	37.67779411713094	43.47525088092853	c
30.85156511177510	35.62694903825894	41.17860681003248	s
31.97427491762295	37.11262277900824	45.41280743983364	h
39.60187168362467	36.84896401816100	28.32450962379954	h
45.14372426786971	24.13175764481732	45.39819668056149	h
45.82113578970515	36.70088367058380	42.38656298064171	h

Table 25: Coordinates of μ -H small model.

7.39706588752833	2.08792601246686	-12.17798239086006	h
6.08479721051709	4.98721735042543	-1.68053989686519	h
2.92533062333052	6.25325738911827	5.29353591061306	c
4.14778451851784	8.01324533111345	5.89440186565717	n
6.73826613518616	0.63209065984092	-9.20318433895593	h
0.57809046065066	-2.77366917535452	2.25339219754974	h
4.51918134566374	-1.93803350159475	4.27301969460094	h
4.93853011719592	5.14464385172944	0.03744282927568	c
3.28803003572183	2.24145724837638	0.96150895366785	s
1.44028272586877	-3.70250297510482	6.00946206677826	n
5.04787077692817	-3.04530683483424	7.44276314371553	h
3.23257181034793	1.13861933849959	7.37868059420265	s
-1.87942938785045	-4.30851843606704	3.96058333283817	h
-2.42085171885423	-1.22767343986092	-1.84554510927790	s
-3.54869955095156	-9.59889226426238	7.35577434152752	h
3.68357197224159	-2.13144998099667	6.16872209752705	c
-0.36423021078495	-2.89605434599758	4.10143170211522	c
-2.18020162547998	-8.66326474910852	8.60196527936543	c
1.06509928734972	-9.53212551207590	7.72052461068633	s
0.89146018306836	3.40655228232165	4.42331540202096	fe
-2.50876022242146	-8.28501888321813	-0.55936589738391	h
-0.94967944250380	1.63863335393610	8.62690708640233	fe
0.34515630344329	3.75042850139519	-5.71741289987153	s
-0.70399163811823	-8.56096803480259	-1.53711045328020	c
-1.03374244116107	-7.77089809624109	-4.91064524220546	s
-0.65741074295783	-3.51701727529641	-4.86616577253904	fe
6.36961208626946	0.53673681846586	-11.24235242992465	c
1.38374738107654	0.76113125146418	-2.72780589926966	fe
1.38830122104469	0.32901510706304	-7.94879436128965	fe
2.97330545602988	0.75668341586975	-11.91558067200865	s
-2.30488762064972	6.69771140756951	1.41984519447922	o
3.51526897563760	6.61931725708463	-0.26877274889635	h
-0.04832813406559	3.50532156328242	11.23010327460208	c
0.46817901676728	4.68432051643691	13.01202488885931	o
-4.36368579323898	2.81205460770648	9.02969973539718	c
0.56349843288074	-3.60439003551219	7.73700606188271	h
-1.95623027029432	0.20197993576403	4.60969041496495	s
-1.06639821787486	5.33597016823995	2.63277579151292	c
-6.43108014910037	3.50873356564013	9.43678023961326	n
-1.63070120705606	-1.03073267513155	10.43116472452761	c
-3.15007487107907	1.04886561368306	-5.54373864691863	fe
-2.44105093499297	-6.61301692796900	8.49674110305876	h
-2.53066585801485	-9.24266527622002	10.56247461733174	h
1.61660656799720	-7.23451994256310	6.53895759670420	h

3.53253182369647	-2.10165601502322	-4.97080751274064	s
-2.43499060124247	-1.80641666152717	-8.48613532950951	s
-2.14717137216853	-2.76554555962831	11.70849719640058	o
0.72175652641441	-7.35564504569645	-0.63341912904135	h
-5.85342554166574	7.88153121268825	-5.93273938643076	h
-0.12153555918550	-10.54803072368990	-1.34316317173697	h
-4.00686284875017	6.25415315168630	-3.62355264308681	h
-5.86423893834657	6.35724885720868	-4.53056777866221	c
-6.66080255438183	3.34744972606895	-6.07988658026645	s
-7.27802302695771	6.78752789183224	-3.06962547537641	h
7.09541965990653	-1.27103667837919	-11.94570213989796	h
-0.63036694591814	4.40384947922052	6.91680837820225	h
6.11373938078373	5.71583093126227	1.64424301121781	h

Table 26: Coordinates of the product of shifting the hydride from Fe_d to the sulfur atom distal to Lys358 in bohr.

39.97967227968847	39.93721705762673	29.65497394985907	h
50.18593236384506	38.71882382750552	52.89088944907805	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.74314784309139	37.19092998684763	31.46835102978179	h
37.17224514674805	20.87863604016891	48.77390097902129	h
32.46842398002293	20.89902825580285	50.83401516317580	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.24849500849318	44.91786006756014	49.76923279594953	h
48.11931912759644	26.85172698246778	42.57390019424022	h
46.89236688187871	42.94040637256639	46.40991791903048	c
47.50148255127750	40.84971412668710	44.84986374416025	o
36.31352031898800	30.50399955279624	40.20119475208109	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.23650849830794	27.70765933657736	42.42505026391474	c
41.75814537964607	26.79501399042750	41.90591974468754	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.58176284209598	19.04809898546649	41.85451248128455	s
42.44924088820191	32.15041027586115	45.50821493224223	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
43.12187072082448	27.74992233087501	48.16273515041325	fe
36.99304283863037	37.15775450893264	38.44136444145710	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.56480272373928	26.47177279378132	34.11567229711520	s
39.23665849598704	33.45216997150614	38.73003226683827	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.16465368179877	30.22309862137000	36.02648188918091	fe
33.92970863639170	33.99730454642948	38.88856150306094	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.27391241130974	21.06698874726976	51.42747808812132	o
42.83444849185575	37.80456342370107	42.55336674243605	h
40.55186276749532	21.97697455087433	56.13614965987672	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.43493718275824	24.53663848404602	43.53488339848330	h
47.55071892562386	39.42925342561166	49.56062410251838	h
50.67067513018419	43.45484216695191	47.95396581867429	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.75879551670059	24.68514880550908	57.13343020885063	h
36.59623282247476	35.36489888186108	34.64270993991969	fe
41.16607372730998	21.23045647814322	45.14409432379447	h
41.57841366163493	17.96477749221573	45.74186093812856	h

43.08964898780656	21.21965657111187	40.59343528455275	h
39.81314736528200	32.35267171192994	34.70612644453767	s
32.92351061086039	32.96498890945181	34.98685045229387	s
45.15459752972109	22.63764960538814	48.81330705087556	o
39.21143040759088	25.20852700640824	36.68436775491202	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.89322051106056	22.59841281799059	34.99171744322773	h
34.52263584549369	37.53255033717382	43.22825267311361	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.81570512602626	35.55274261855669	41.28098680156345	s
32.01407623239009	37.14397831451556	45.43133022658491	h
33.64126222046876	28.79330215928806	44.86688108612188	h
35.71245622926616	29.60421225752353	47.40320967649341	h
32.37473281274727	24.98439311487136	47.81852246680452	h
35.29831249461780	25.70383108692200	49.26654808597227	h
35.24705206872692	24.93797207839820	46.25860646897279	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.21999778497181	25.87424472404475	47.60692531393592	n
34.63015776099778	18.70056597133140	48.28270812889641	h
37.37106043665225	24.46709166037992	54.23170199006477	h
25.25802995521681	20.43297772419662	46.90574705299414	h
24.73812166576265	21.18789690794428	50.12670474934167	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.45076633672830	22.23551288363621	48.71234126051532	c
29.42548053938086	24.27061157584502	47.89228526413967	o
29.58145623522808	20.41659369728339	49.77383845192662	o
45.90999191191969	36.50600779315593	42.21363345306758	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.61544633150114	28.17364967821540	40.35614773123558	h
46.13860335284249	29.14419878717841	40.92701652377951	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.15466118103619	37.84363405748663	31.18562413044694	s
44.93403389351462	42.80060625573738	47.13487278748839	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.00076006083257	44.65830050234074	45.23335740835148	h
46.77862463062984	39.29549618676593	45.64140986249655	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.71473648424710	33.40193487871412	41.36417048729776	s
44.33162939211816	25.83580629205320	42.09649759315770	n
45.66755776739088	29.57476451130351	45.45615242508426	s
40.48024183191136	25.21373492294104	41.48636224380028	h
40.42555501916573	28.37146128792991	44.77980101728775	s
39.66152173782157	33.65721702604426	46.40658063114501	c
37.81811594781207	34.70761590297290	47.00177716882438	o

44.32826714656991	34.86955260306520	46.85288511568322	c
45.54452303122633	36.61490125252278	47.55010280652364	n
44.27415228165989	29.40277943944334	50.82045528379682	c
45.04942888356495	30.41118330959263	52.62007747471826	o
40.16615189014854	26.94328676629658	49.95946504568168	c
38.31449357121911	26.30940151716280	51.02650746942045	n
44.30100272195039	24.65636382831448	48.46732591976081	c
48.07044308088805	30.33764674265677	46.02946290990498	h

Table 27: Coordinates of the product of shifting the hydride from Fe_d to the sulfur atom proximal to Lys358 in bohr.

39.87953097488106	39.95759390935396	29.63655979887003	h
50.18748462239685	38.71824617402126	52.88819905326007	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.81371048964462	37.25706060760560	31.43599046998934	h
37.17288583997549	20.93009846901794	48.84425364569817	h
32.43818766165316	20.84292555872143	50.73959104479670	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.26530801365234	44.91695575074636	49.77803109215172	h
48.14774331892006	26.49376527453103	42.83927037508097	h
46.87867539842756	42.96358536563943	46.42041758960927	c
47.48404861843824	40.90232328031032	44.82236258820186	o
36.33044495354864	30.37876065245113	40.30189290211953	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.33518893992717	27.49728572011403	42.72019553884465	c
41.91274625823978	26.74352334582796	41.74182439777963	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.55442191092686	18.99835921172091	41.81170720372764	s
42.61866070385547	32.12504616307641	45.42707156643171	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.85357493222993	27.87184233408330	48.11819405420200	fe
37.19105004643112	37.02185331781666	38.52394951617144	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.52556929174945	26.43421090787185	34.11422310215806	s
39.35382704514104	33.27434564521847	38.80843388570511	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.21670283864152	30.12130872575591	36.08529021100230	fe
34.06294199822188	33.95189528594211	38.95921280515091	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.20509448472519	20.98921077873736	51.42939971983088	o
42.69736372115758	37.69939893526317	42.50929397496961	h
40.55129679795353	21.97609078756870	56.13626919294201	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
44.16647200500677	24.61119423069468	43.95314622002089	h
47.56860211155410	39.42162078446531	49.54742213188261	h
50.66697304913415	43.44905656213177	47.94072165548678	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.75868877063642	24.68217932504282	57.13545092186570	h
36.76788503655242	35.25083176944477	34.71854971882733	fe
41.17300233435078	21.25648179996208	45.08378106470315	h
41.55212311967406	18.00980974913110	45.79025107116131	h

43.87376657135574	21.49083910599758	41.25521837893774	h
39.90107426962784	32.15176839011166	34.79449893362919	s
33.03609999242494	32.92346527513588	35.07439582251175	s
45.43332635561315	23.15390374530298	49.37994268982929	o
39.20221731429213	25.23121206147955	36.67456996880710	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.91464114965942	22.59756255868194	35.00389271645201	h
34.53048338970387	37.54283001518627	43.29314737600656	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.89372044286879	35.57154950937075	41.21244296443957	s
31.95541983142490	37.12536600325025	45.41125815216112	h
33.65943164257702	28.86325057914943	44.87069484872980	h
35.71982763680581	29.55052211266559	47.48883719120978	h
32.22516318817272	25.03298258521101	47.83231550444008	h
35.25711185495827	25.61998088019713	49.18124543221514	h
35.02079465721056	24.85540631229792	46.16274461579836	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.11735967738284	25.85035464917859	47.55448395007615	n
34.68464424701576	18.71451713517436	48.23311109915836	h
37.35183897360024	24.44157920389631	54.22288314215676	h
25.20922631342231	20.40103935762421	46.95169783150076	h
24.78782391385904	21.23309162372224	50.16690214675439	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.44916725922025	22.24216459035946	48.63122465897538	c
29.35692171549642	24.37682426484757	47.99245513542847	o
29.64745406081148	20.35338416380154	49.46135320983226	o
45.88063123310713	36.63807148956162	42.27464598596185	h
39.60263513297916	36.84967455518400	28.32505575464967	h
42.01415604478034	28.06664575798175	40.14415042748379	h
46.36868557897863	28.82793017681075	41.12274730773049	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.19267887577943	37.70004598482362	31.27057320751404	s
44.92573462364160	42.80630990028809	47.15849588713267	h
44.15850781758571	37.44327910501924	39.48682704686118	h
46.97179173183611	44.69910668156815	45.26840455299720	h
46.82331228200002	39.32613455741209	45.62605872290940	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.98683329235804	33.31391628085572	41.29418065764051	s
44.33230637108716	25.64678351339625	42.30955480995446	n
46.13435996962409	29.48576078841938	45.64616816681531	s
40.49030824679870	25.28366017822896	41.35674837814646	h
40.75097631234664	28.56212063901294	44.56378084296855	s
39.87848789028905	33.79089727125182	46.13936959102752	c
38.04523567700652	34.91436369950453	46.63923439455988	o

44.51697260332615	34.83855538169315	46.80453862407639	c
45.64858553630140	36.63118783826114	47.50896774458335	n
43.54984214877819	30.11244843880172	50.49606615357416	c
44.02876059530146	31.36375551039905	52.24478707712839	o
39.96395952924673	26.85914870463476	49.88807109927645	c
38.13444117183321	26.13336807637524	50.94317789790804	n
44.34385880110973	24.99802236240924	48.80293322619993	c
38.27100974750000	28.80416317998432	43.77067000541606	h

Table 28: Coordinates of \mathbf{O}' without Glu361 and Ser323 in H_{red} in bohr.

39.85136077502784	39.96234063803925	29.62708433865863	h
50.18770212651763	38.71615304335342	52.88472906607694	h
50.26532597612761	40.64384966141100	52.02713464999426	c
51.72791730508891	42.27462094631834	52.76220787699877	o
40.83334462396656	37.27379276649676	31.42391258607552	h
44.08943215813802	25.57487482505075	43.08937693429203	n
40.24669655342181	25.14987819316023	42.22581717688168	h
48.55707969954778	40.96887121655315	50.21873477851589	n
48.71770075099387	43.22511728239375	48.64276366150725	c
48.18762673002019	44.91110666391201	49.75492954109738	h
47.93640028647359	26.46007614283262	43.23648134424996	h
46.97166517154165	42.93134866183461	46.34921909723712	c
47.69942984050797	40.90730030934545	44.75978969437845	o
36.40761101217014	30.44311286757454	40.27262753915041	s
39.24105115677064	18.94452330032199	43.50905052240016	h
46.10933257751009	27.44280481542883	43.13442517986731	c
41.62245840495618	26.67011556665901	42.56343977031167	c
41.12452228829050	19.35004718838886	44.26890561780783	c
43.45993748556242	19.51593544571020	41.69837034875063	s
42.52902253822154	32.29787801064103	45.67674129542318	fe
36.36718023232001	23.76148999498827	37.77248262407600	h
42.95877959362954	28.31519221024145	48.59888748657138	fe
37.16834914848406	37.14821500481844	38.53924353276591	s
37.43969996373850	24.30660984163455	36.08670897057459	c
35.60770642138927	26.56683027335747	34.17785589692067	s
39.25111997198178	33.38589088181791	38.79251238460114	fe
46.09010690631604	29.73383522511319	45.82569556173800	s
34.18174880210214	33.96729488548775	38.90029320364663	fe
36.77798323387762	35.24561040657216	34.82248665720351	fe
40.29393576336625	28.64712127162849	45.14077047625247	s
39.83232392279655	34.01309329711748	46.41330254337396	c
42.82275784192384	37.80069322080003	42.54540684781024	h
40.52666436888948	21.92967499167372	56.13327907541782	h
38.98732518887225	22.68717502375104	57.35097313453696	c
38.83615087832501	22.33192163006125	59.63556509225246	o
43.99998979831498	24.82410887042309	44.89130938085966	h
47.55689487829032	39.42324826141969	49.53362047199822	h
50.68563658107719	43.49200945588257	48.01316995798918	h
37.24884518401865	24.02694171349225	56.12459001229536	n
35.97416678120283	24.95054183316901	57.22494691458873	h
36.32437118069145	30.30501703058761	36.11456542883536	fe
41.07179950073972	21.15041855986407	45.29580635489271	h
41.66614821996990	17.85823384828821	45.60426720827225	h

43.95509037727419	22.09399590395304	41.86694976370022	h
40.00206109889643	32.31469463556090	34.80598554219097	s
33.06318322245006	32.96158204845765	35.04835337840447	s
45.89452575086520	23.93539476493197	50.27507982748312	o
39.24181733823037	25.13404747728460	36.69361657027897	h
31.89727118913942	39.64356849057265	43.16713103624832	h
37.83234559279199	22.60630886904794	34.95504132931311	h
34.53441692419225	37.55649129730536	43.33773264402622	h
32.47179895374285	37.67779411713094	43.47525088092853	c
30.96532829107564	35.54337995700025	41.18428369549442	s
31.92644262612730	37.12394644311532	45.40397431961471	h
33.57678612419486	28.80111288454994	44.86603637173913	h
35.59621828313313	29.83264896106846	47.29372158727677	h
33.14609367489822	24.80225980313502	47.41272544576812	h
36.62163109879933	26.17898010000432	50.10111238070134	h
36.03335646132068	25.41643011015715	46.42324398889049	h
32.35447908672487	29.36437866723039	47.94215148011812	h
33.97407453132900	28.60368075397097	46.89930233858816	c
34.64268641842193	26.00082018248341	47.64540677531754	n
38.04490531519934	35.19951915160413	46.94775761351685	o
37.62881997201192	24.78753042594289	54.35427108595287	h
44.51132191473913	35.03872171142828	46.82100791236950	c
45.70671874419190	36.81383032443900	47.47319235311883	n
43.47285134267317	30.94373983603844	50.63112177207403	c
43.77684901266072	32.37912871319303	52.28182736078717	o
40.22747103168725	27.28512713444651	50.20950546622487	c
38.31639521485221	26.48940636118648	51.21977119299408	n
44.70240394634337	25.66243570194089	49.53757570846692	c
45.90963001756808	36.53108074917288	42.21299627779492	h
39.60187168362467	36.84896401816100	28.32450962379954	h
41.71034974971680	27.85376005674108	40.85731803392319	h
46.01919676067563	28.58618395765896	41.39920825310814	h
39.43517138323448	37.96880060202321	30.05871317843228	c
36.21017256843663	37.64717027990751	31.30326444261549	s
44.99808050222130	42.70421403880594	47.01039854704985	h
44.15765555110334	37.44255722963949	39.48606548723281	h
47.05502734895560	44.68669474062280	45.22424113867510	h
47.01051158004307	39.31965181116281	45.53052456007870	h
44.02135905433818	36.58935344310939	41.36828939951017	c
42.76240304453975	33.36729478720170	41.45353243491972	s

Table 29: Coordinates of **TS(O', μ -H^{Lys})** without Glu361 and Ser323 in H_{red} in bohr.

16.03789701002366	1.64932721220270	2.03966642114055	h
-4.55829324609015	15.94149301547117	-2.02014915541102	h
-2.75069479617129	16.86509512854479	-2.60083195555480	c
-2.56373285226893	19.14901812321204	-2.89583710092755	o
12.88570701164097	1.12177554224961	3.14290727909619	h
-2.36701181636284	0.96370438749833	6.87848541481756	n
-3.21337702795947	5.12298364687256	3.52321917950085	s
-0.90857465171854	15.21581019679089	-3.02482980621961	n
1.65342532169377	16.16534277254254	-3.39060519497337	c
1.71550394474705	17.40247662161121	-5.06394826989643	h
-2.47075001489440	4.73587648802981	7.99053260978661	h
3.40535942482908	13.86721009766862	-3.71705430930061	c
3.36209197465057	12.24395719138931	-1.59253871678360	o
2.61911561023277	-3.24795879871544	-0.42612997951449	s
-7.22468753750799	-6.90749889715394	6.32795390968866	h
-1.79646669448306	3.58522040878492	6.39812847724541	c
-1.45586108178490	-0.73633929116311	4.94392825881120	c
-7.81766280854361	-5.03435511890717	6.98255503938644	c
-6.29232425549227	-4.19761642954795	9.97518267167077	s
-1.40485610914342	3.34492242294517	-0.08695470992263	fe
0.52567834427234	-8.01540752971519	4.57654628841397	h
-6.29412139465405	2.45753998980680	1.95734559824534	fe
7.86864307809404	0.64608711536416	-2.88587214789543	s
2.07761403469720	-7.44778860382474	5.82478787274337	c
5.14437130266008	-8.20779632178419	4.36156015319209	s
5.31011299516935	0.07477011330775	0.51329784482941	fe
-1.89323455717370	-2.69870991501061	5.47582067703873	h
5.97797175755556	-3.28492036453498	-3.25433217816304	fe
5.78870803341961	-4.93660752726622	1.69556572396302	fe
-2.82137152565667	-0.35250633744711	1.72010753768121	s
-0.28237416398165	2.66254676931641	-3.07634767662809	c
4.07123651321394	6.70218297567483	-1.27442393991225	h
-15.80046606010264	-0.09881315113823	-0.73379724671820	h
-16.17584776007138	-0.38759983577131	-2.78327178484006	c
-18.20580479162237	0.02954964741652	-3.81915161642105	o
-4.29293761316381	0.76377772290175	7.02122013416598	h
-1.15657708423748	13.34732534736147	-2.54845612612310	h
2.23375465629175	17.29183740917761	-1.73611848618160	h
-14.20986551675592	-1.26734860517920	-4.08000941071516	n
-14.41935071120020	-1.38127062856324	-5.98333897131906	h
9.81056930720846	-2.00283922628537	-0.28169853877440	fe
-7.42361229560674	-3.60024484384717	5.53636537940872	h
-9.85818575759262	-5.03691929803976	7.34598473116553	h

-4.01846238373422	-3.52015464391058	9.01924406715740	h
7.79008602666422	-1.42544253960720	3.53857926654975	s
8.59504790821169	-6.00737280321976	-1.52653902503426	s
-9.58044108911829	1.57977641243503	6.31801790196591	o
1.92641096710303	-5.41192169537121	6.18705768293929	h
5.91639612610468	-0.11490290730411	-9.90827437952851	h
1.90924878710165	-8.46745787096756	7.62985902967254	h
4.31682700007085	0.59607164399808	-7.03397402842107	h
4.46037915433224	-0.76119491123029	-8.58497287351438	c
5.19660441268612	-3.93220126015902	-7.37317364560478	s
2.63157510231428	-0.79812922299641	-9.57404348468486	h
-5.23110321325255	-4.84407266162069	-3.11799248245502	h
-1.87292236460928	-4.55871140268977	-3.58062775530373	h
-5.78919941839100	-0.65755226460243	-3.46716245925603	h
-3.56129642615831	-0.26986815707432	-5.64897548465678	h
-2.51849016152770	0.98044287455901	-2.34551040666382	h
-3.95432750559409	-4.34448792026476	-6.25639942996578	h
-3.74172575762781	-3.94256773991825	-4.23599118452438	c
-3.96789967095233	-1.12060423102775	-3.96455358114034	n
0.55338130109870	2.50462277328955	-5.13465541813909	o
-12.40045935358841	-1.32328431757775	-3.27554529268733	h
-1.27069019203709	6.77049468372321	-1.27508974857057	c
-0.907471110522380	8.88317516265828	-1.91007868835554	n
-7.87605135240061	5.03679669341492	0.56981735864046	c
-9.02806975154029	6.69468064124813	-0.32472065090898	o
-8.19340585550036	0.29988139631788	-0.17796473449394	c
-9.42088904853827	-0.98329937544366	-1.53625752500253	n
-8.17873618821556	1.85627921693362	4.61272989939889	c
3.17905633058731	7.93234187307691	1.73035306101627	h
15.36928997321061	-0.91205930669303	4.14335303042495	h
0.60423067342828	-0.55706945218268	4.73189798081028	h
0.25824867712883	3.81653697669827	6.17186056507172	h
14.64139581575496	0.19255742295847	2.54999454334023	c
14.08918984303569	-1.93104462348180	-0.14157562038812	s
2.87065491537292	12.85130963252292	-5.46691357938789	h
6.19688061593298	6.40694635143952	1.32022125243040	h
5.36336441887758	14.54510250928251	-3.96105101084597	h
1.95160642637464	10.99291638720395	-1.75579980444528	h
4.20022433815663	6.40870001728351	0.77051315075264	c
2.66701352151911	3.39091109104622	1.60040100869157	s

Table 30: Coordinates of $\mu\text{-H}^{\text{Lys}}$ without Glu361 and Ser323 in H_{red} in bohr.

39.97090086609946	39.93667417635196	29.64994807131512	h
50.18891841031220	38.71322262918405	52.88097338973800	h
50.26338711712337	40.64228118872726	52.02512776084952	c
51.72592175430091	42.27298822294635	52.76017075223603	o
40.75153047972977	37.19458816232062	31.46023151560324	h
44.05468382849071	25.80125722970234	42.51229413410494	n
46.15605995599363	29.76213997864213	45.52601804653640	s
48.55520509123179	40.96729140551265	50.21679591951165	n
48.71582236322562	43.22345054395151	48.64088527373900	c
48.14401870360799	44.90543857848404	49.73811580183094	h
47.86652173377424	26.77581250813700	42.53666866644686	h
47.01576161157338	42.90476916669721	46.31703435417892	c
47.78681586744578	40.87267303566987	44.75375114459685	o
36.36375476016655	30.53556720127505	40.23042738289528	s
39.23953559641839	18.94379386603774	43.50737244560116	h
46.01189005306504	27.70215522866682	42.64271236880690	c
41.50926145177139	26.79816952531370	42.39617121707736	c
41.12293491834551	19.34929885684336	44.26719730539084	c
43.54442309500399	19.21610322956927	41.78515314711978	s
42.56702085711618	32.29850949557413	45.61328326185266	fe
36.36577805553527	23.76057158809153	37.77102375550750	h
43.23905286331437	28.29716129463743	48.42653149273223	fe
37.06088669665163	37.16775426301567	38.47664034035515	s
37.43825621297900	24.30567253747655	36.08531813214660	c
35.57687233129227	26.49840161722866	34.13031639085463	s
39.29514913023377	33.44800567006212	38.76780512277244	fe
40.15504680769045	25.23743520873160	42.19461097691801	h
33.98249806531476	34.01856142414611	38.91022683752475	fe
36.66160727824123	35.37692100102341	34.67573783509182	fe
40.36952199778479	28.64627054722088	45.16133277075079	s
39.83899849558212	34.05306952078510	46.16845478127766	c
42.79596523350121	37.78337427771906	42.53390274039785	h
40.53308405346765	21.93733280316549	56.13420032929650	h
38.98582096687675	22.68629819082905	57.34875837551846	c
38.83465043578177	22.33105991494825	59.63326340583222	o
44.21444411621440	24.65778510714996	44.06554063730125	h
47.56413339207182	39.41864068391226	49.52942555283881	h
50.69176467498082	43.51284574567192	48.04875799950325	h
37.24740899216365	24.02601574769100	56.12242438615612	n
35.96962472385422	24.91207389127554	57.25229932808477	h
36.21975942760578	30.23610306715955	36.05975888385499	fe
41.11543954055934	21.20220818764937	45.18875264495353	h
41.61421859060746	17.93124068266209	45.69690437942987	h

43.62523500683064	21.73415886471307	41.23124704297219	h
39.87134633513124	32.36305475049464	34.73663525825397	s
32.98111886578910	32.98343323653053	35.00924751618949	s
44.51924399440787	22.94258325393075	48.59581936030138	o
39.21596683284225	25.18655403496706	36.69059507809816	h
31.89603908770593	39.64203781241140	43.16546429780607	h
37.87863360261714	22.60110222038104	34.97815355045096	h
34.52227515818441	37.52886445772144	43.24424543148766	h
32.47054417559585	37.67633902801470	43.47357280412952	c
30.82325329464266	35.57379794143222	41.24830502240435	s
31.99622002984026	37.13056680964260	45.42195534490362	h
33.56012179628661	28.77405662944040	44.86662405643985	h
35.60321602079653	29.82508445207256	47.26553794168146	h
33.05064284456584	24.95295825609930	47.92967272666923	h
35.73661913671209	25.97033626178250	49.13744992446495	h
42.46847381258535	31.47564271493290	48.61407080891983	h
32.35323186748238	29.36324483155540	47.94029954851563	h
33.97276306139826	28.60257715391398	46.89749198096042	c
34.64146932488629	25.97483429430352	47.54087179423487	n
38.05473341844976	35.27799575039577	46.56969026659701	o
37.66564320618509	24.92712377425849	54.41027208875961	h
44.56162385330212	35.03137079055813	46.79267947285808	c
45.76065124326126	36.77298228456853	47.51571623006458	n
45.16556543280605	29.08445011155699	51.03425030182243	c
46.38242646078230	29.56516070432404	52.79695470541122	o
40.43470962495479	27.63849990053621	50.57999898805136	c
38.75890256659829	27.02755217787312	51.90432440196832	n
43.99153721849490	25.08405695610054	48.45522140687995	c
45.90423996996181	36.54956103168393	42.21972105470358	h
39.60034478491567	36.84754294411501	28.32341736209930	h
41.30733830047158	28.05201106010927	40.75021382238025	h
45.78864802885896	29.02426432036601	41.05164794228920	h
39.43364826397773	37.96733417455021	30.05755288659154	c
36.15820007484677	37.82722219055644	31.19884296536464	s
45.03058083531897	42.67030499536790	46.93807959964977	h
44.15595101813859	37.44111347887999	39.48454236797606	h
47.11227111021022	44.64992572922298	45.17927065396966	h
47.10340260053469	39.28997624868568	45.52411789372526	h
44.01966208027793	36.58793992796789	41.36669447066068	c
42.79747375892837	33.37148979507216	41.39012385277383	s

Table 31: Coordinates of O' without Glu361 and Ser323 at H_{ox} in bohr.

39.70748855252351	39.97987569806623	29.61212174738032	h
50.18206247277992	38.71969110586557	52.89363665959174	h
50.26532597612761	40.64384966141100	52.02713464999426	c
51.72791730508891	42.27462094631834	52.76220787699877	o
40.90577556929044	37.36939567656834	31.39030418642339	h
44.35822147154303	25.63046284410476	43.04384085074329	n
40.57464128411831	25.05464322757143	42.05226009236716	h
48.55707969954778	40.96887121655315	50.21873477851589	n
48.71770075099387	43.22511728239375	48.64276366150725	c
48.43243898747891	44.91876891581082	49.82332494441250	h
48.14547666972158	26.63726743674587	43.46155883903639	h
46.72685978147902	43.11287347900852	46.54477043834785	c
47.13416777925682	41.10437945758819	44.81496401476449	o
36.49446355136694	30.52335842116701	40.34692205432723	s
39.24105115677064	18.94452330032199	43.50905052240016	h
46.29945081141956	27.55627465439893	43.22375504925144	c
41.87779602197886	26.62419078937166	42.44588921812554	c
41.12452228829050	19.35004718838886	44.26890561780783	c
43.44812373536591	19.36973014737530	41.67987252493720	s
42.41820829245822	32.25931542752473	45.56749037329045	fe
36.36718023232001	23.76148999498827	37.77248262407600	h
42.90887498610790	28.38518989595974	48.54129731318554	fe
37.40641198882752	37.09069067724369	38.54837437913226	s
37.43969996373850	24.30660984163455	36.08670897057459	c
35.62218572780386	26.63474558565897	34.25445453345230	s
36.95810047319438	35.15700394434936	34.81355625588690	fe
46.05821914198928	29.87072506435327	45.89293892194047	s
36.42104783974966	30.28851463482514	36.16695327344211	fe
39.29109905992197	33.33415978679436	38.80305013506727	fe
40.36797050982269	28.52700797372808	44.99305898494364	s
39.68174949935323	33.83267723396409	46.53138958115331	c
42.89105042543827	37.83261092479686	42.57658333997022	h
40.52619042322375	21.92507599070918	56.13389697028587	h
38.98732518887225	22.68717502375104	57.35097313453696	c
38.83615087832501	22.33192163006125	59.63556509225246	o
44.24386374438802	24.76666348756381	44.78538868291386	h
47.54412766046291	39.43674569171237	49.55747534431701	h
50.62147666907514	43.36580491326188	47.80651557908863	h
37.24884518401865	24.02694171349225	56.12459001229536	n
35.96401653202980	24.94441566315131	57.21822605708418	h
34.40550275721554	34.03710215453874	38.91780489423326	fe
41.09809010347499	21.18944814739096	45.22368965767489	h
41.64388275951745	17.90091808332203	45.65649039726251	h

44.10040388900615	21.87760625005363	41.80639889608701	h
40.07358098566702	32.21248777503405	34.88411081180214	s
33.22540365341777	32.97883368335638	35.15248975442073	s
45.67308548245002	23.83548263763836	50.04536726286300	o
39.27191846583735	25.07856519891173	36.67285282330804	h
31.89727118913942	39.64356849057265	43.16713103624832	h
37.76133535516651	22.62665056901077	34.90884451208754	h
34.53990361779062	37.57569960469375	43.48756613556293	h
32.47179895374285	37.67779411713094	43.47525088092853	c
31.15830059333313	35.58099901388134	41.04650779232780	s
31.78845946474539	37.07161219064999	45.34089011798705	h
33.56283376336659	28.76368804547527	44.86738389257013	h
35.60348174115589	29.82716101726922	47.28150059282728	h
33.06553249517886	24.84592369524813	47.63523061086771	h
36.46723516026834	26.23900542831043	49.98734107025183	h
35.90184155510408	25.30705655983200	46.41301168260575	h
32.35447908672487	29.36437866723039	47.94215148011812	h
33.97407453132900	28.60368075397097	46.89930233858816	c
34.60995412917025	26.00324511023362	47.68029780906925	n
37.87959872443615	34.91534365281638	47.19907683208309	o
37.60179899710180	24.76240259463250	54.35456306871240	h
44.29566543834491	35.04044844204298	46.82847876726073	c
45.44336124752613	36.81936523070048	47.52871735746533	n
43.60095536923605	30.74055524015825	50.83116916655379	c
43.99821079023597	32.12360058953885	52.49082296925946	o
40.10788046009451	27.41084773224523	50.14102433847488	c
38.20071583046337	26.61958184124693	51.11408954227459	n
44.53873865021921	25.61494870459464	49.37703273606526	c
45.91380448878854	36.44203033674800	42.19523492374287	h
39.60187168362467	36.84896401816100	28.32450962379954	h
41.98051248453518	27.83210953254621	40.75685297840278	h
46.30145096679542	28.68956111070725	41.48142014623353	h
39.43517138323448	37.96880060202321	30.05871317843228	c
36.25738859179321	37.47208473986458	31.36564810416429	s
44.82307433005498	42.99621862499223	47.40891330280141	h
44.15765555110334	37.44255722963949	39.48606548723281	h
46.81128807110255	44.88868303275711	45.45717403758619	h
46.54213822788085	39.51524404023874	45.63414205715938	h
44.02135905433818	36.58935344310939	41.36828939951017	c
42.65409825539248	33.41248217393787	41.48782548115788	s

Table 32: Coordinates of **TS(0'**, $\mu\text{-H}^{\text{Lys}}$ without Glu361 and Ser323 in H_{ox} in bohr.

16.05694834765947	1.60157215182281	1.97949650834983	h
-4.55957172752559	15.94234823442170	-2.02079519049098	h
-2.75069479617129	16.86509512854479	-2.60083195555480	c
-2.56373285226893	19.14901812321204	-2.89583710092755	o
12.91361739741625	1.17085054772041	3.14230104281838	h
-2.15845563410806	1.08841222936955	7.00230280311747	n
-3.34434389893385	5.09847141704827	3.53814820723665	s
-0.90857465171854	15.21581019679089	-3.02482980621961	n
1.65342532169377	16.16534277254254	-3.39060519497337	c
1.68814422773313	17.46835053881721	-5.01174847636790	h
-2.60399550009315	4.84864654204792	8.01462820842263	h
3.40122824354200	13.89278839217848	-3.84736518146026	c
3.41101767292421	12.16272587649922	-1.79343826648228	o
2.60975840060911	-3.20990942374471	-0.39264721082745	s
-7.22468753750799	-6.90749889715394	6.32795390968866	h
-1.81862157226011	3.71886168299583	6.46177924728452	c
-1.21997863188382	-0.62240288452067	5.11602168841029	c
-7.81766280854361	-5.03435511890717	6.98255503938644	c
-5.99395700056691	-4.06100466290233	9.75579538611570	s
-1.38174682496425	3.30641553326074	-0.00151235854181	fe
0.52567834427234	-8.01540752971519	4.57654628841397	h
-6.24816372807992	2.26983982232926	2.06007436379472	fe
7.71754035834514	0.62085670044918	-2.61396663308994	s
2.07761403469720	-7.44778860382474	5.82478787274337	c
5.13178657222138	-8.20351604709130	4.34125690020427	s
5.78123637805209	-4.96267601385793	1.75149268181694	fe
-1.56008638611778	-2.57880575992740	5.72045166444918	h
9.84182805152420	-2.05847688877572	-0.07116240878346	fe
5.11924663823224	0.13473392727631	0.75682072246850	fe
-2.67897303081988	-0.41183056923145	1.90303566590075	s
-0.29480921072214	2.56569896459141	-2.99537842475659	c
4.06137924207432	6.64406061244858	-1.28027014316974	h
-15.79972773278653	-0.09482717927673	-0.73388855494585	h
-16.17584776007138	-0.38759983577131	-2.78327178484006	c
-18.20580479162237	0.02954964741652	-3.81915161642105	o
-4.00853546323713	0.68698995374749	7.40493045122319	h
-1.15869155143527	13.35898273541043	-2.53080258925131	h
2.26732227696319	17.22465352042776	-1.70422040052964	h
-14.20986551675592	-1.26734860517920	-4.08000941071516	n
-14.42053683588816	-1.44869470868642	-5.97702701800833	h
5.89377706577709	-3.27328115599908	-3.25418513768274	fe
-7.62620739415394	-3.65307225803136	5.44735067751550	h
-9.80003829363730	-5.09676322520037	7.57994885441319	h

-3.67344301508134	-4.35299666529652	8.72344405661691	h
7.65581917281190	-1.50786041118381	3.64027897686355	s
8.47847932114461	-5.96168320535460	-1.50019589071654	s
-9.28200443648970	1.34379858123520	6.56897944159574	o
1.93842531273624	-5.41533088252091	6.20569117928505	h
5.91639612610468	-0.11490290730411	-9.90827437952851	h
1.93548542841480	-8.48579775282201	7.61822396698024	h
4.28657970979163	0.61679134661942	-7.05573405772657	h
4.46037915433224	-0.76119491123029	-8.58497287351438	c
5.18779689954338	-3.89970684937270	-7.30903008507741	s
2.64153683471457	-0.84183765115279	-9.58386530660945	h
-5.18672995260954	-4.91422002009284	-3.11866440396668	h
-1.84953548407730	-4.51208198486888	-3.60427063865626	h
-5.89295420981476	-0.75306037801401	-3.41175621080974	h
-3.69775913538102	-0.25099185187115	-5.59769125415632	h
-2.63255989028277	1.07340195195564	-2.21199088326964	h
-3.95432750559409	-4.34448792026476	-6.25639942996578	h
-3.74172575762781	-3.94256773991825	-4.23599118452438	c
-4.06165832619555	-1.14184062339408	-3.92494709986817	n
0.53167733872939	2.32833215384365	-5.04289633606921	o
-12.43872744755253	-1.44306591050290	-3.25749844504507	h
-1.27480721842152	6.70580509665749	-1.25784120068118	c
-0.93318447743405	8.80239048559259	-1.93396064575692	n
-8.11426735762965	4.73255433933261	0.78857778825247	c
-9.41982766381432	6.29749810346336	-0.03138266814803	o
-8.14024507734526	-0.00338759016461	0.01367700243483	c
-9.37496819945816	-1.31694950641495	-1.29905620996324	n
-8.01328515971552	1.64582834482846	4.78184727895576	c
3.18412205379233	7.96299240015472	1.68498102895734	h
15.36928997321061	-0.91205930669303	4.14335303042495	h
0.82428413802747	-0.36049724136936	4.83910519448141	h
0.20541297196135	4.13258655246212	6.23462545015679	h
14.64139581575496	0.19255742295847	2.54999454334023	c
14.04199468122957	-1.99066561521791	-0.08861798956133	s
2.84309351717422	12.95040374165882	-5.62969990442072	h
6.19688061593298	6.40694635143952	1.32022125243040	h
5.35304149806889	14.58151427112205	-4.08543488227992	h
1.96094000369154	10.97475052821068	-1.94390705448356	h
4.20022433815663	6.40870001728351	0.77051315075264	c
2.60400339274639	3.45579630391288	1.68199597227513	s

Table 33: Coordinates of $\mu\text{-H}^{\text{Lys}}$ without Glu361 and Ser323 in H_{ox} in bohr.

39.89411698629305	39.95148561270189	29.65045575243588	h
50.17744461415484	38.71976850067369	52.89577512824891	h
50.26338711712337	40.64228118872726	52.02512776084952	c
51.72592175430091	42.27298822294635	52.76017075223603	o
40.77250020187569	37.23917876617401	31.46166342433010	h
44.36316115281084	26.11070866867779	42.02400869395774	n
46.09080772924402	29.96233684952566	45.42476755045489	s
48.55520509123179	40.96729140551265	50.21679591951165	n
48.71582236322562	43.22345054395151	48.64088527373900	c
48.47094030397631	44.91750463190640	49.82856303370941	h
48.09342002361170	27.26498506756294	42.35185281674872	h
46.68485069007890	43.13287066710946	46.58077666404716	c
47.02834757777870	41.10864398010531	44.85279038871381	o
36.36187271086443	30.65075978073236	40.18888175338559	s
39.23953559641839	18.94379386603774	43.50737244560116	h
46.18658540887693	28.07913910943488	42.40768380341644	c
41.76423927789973	26.89387895404677	41.96485982761223	c
41.12293491834551	19.34929885684336	44.26719730539084	c
43.52997514758022	19.35313045361903	41.78649997625297	s
42.34379436357074	32.25599289894652	45.51660687907519	fe
36.36577805553527	23.76057158809153	37.77102375550750	h
43.20325421192921	28.19531989756993	48.14225575572448	fe
37.12843173463210	37.09908073128395	38.36282941045756	s
37.43825621297900	24.30567253747655	36.08531813214660	c
35.57411835594607	26.51510820015275	34.15856264278455	s
36.66644628322180	35.27943756361682	34.52560820170640	fe
40.54144716844120	25.24411083860724	41.65564452120239	h
36.19947064376453	30.21913650957649	35.99611990835039	fe
39.28950322454983	33.44254987183153	38.74403910700953	fe
40.40905585240294	28.46039743395274	44.82993438099781	s
39.51293043338182	33.83016468974502	46.18355544596240	c
42.95769751941959	37.86855376918938	42.59783690314843	h
40.53008322835741	21.93360759748444	56.13143182798598	h
38.98582096687675	22.68629819082905	57.34875837551846	c
38.83465043578177	22.33105991494825	59.63326340583222	o
44.62894767750696	24.65594911134951	43.26613288147966	h
47.53498491907885	39.43932082732360	49.56360162963106	h
50.60554399730223	43.34161626519648	47.76998253847047	h
37.24740899216365	24.02601574769100	56.12242438615612	n
35.94920438065650	24.90970004540811	57.22811903207360	h
34.03071847204146	34.09828429628048	38.87536002761878	fe
41.09726306278609	21.14605022394188	45.29487226307308	h
41.66913036451110	17.85164123804183	45.59115314132536	h

42.68605725022715	21.39561671544970	40.49964995748879	h
39.82067458778124	32.30692690069265	34.75623514183206	s
32.98823236254975	32.98037386210046	35.05483256704344	s
44.80935979764332	22.93400018760496	48.00978326784895	o
39.23084200152359	25.16904488620802	36.66898382823480	h
31.89603908770593	39.64203781241140	43.16546429780607	h
37.83980082306724	22.61436829413938	34.94917930816014	h
34.52936284108972	37.53439294075068	43.32594978329984	h
32.47054417559585	37.67633902801470	43.47357280412952	c
30.92558065363014	35.57093762900966	41.19248997156625	s
31.92225146070278	37.10235549079962	45.39140856995223	h
33.64481912487645	28.97685992423596	44.87563031860022	h
35.64843343923624	29.69622082705961	47.43928812526079	h
32.83546058391025	24.93631776425853	47.60005904735169	h
35.56262287731840	25.69975822313883	48.91115615222845	h
42.24544405556554	31.30019544479302	48.46920712230910	h
32.35323186748238	29.36324483155540	47.94029954851563	h
33.97276306139826	28.60257715391398	46.89749198096042	c
34.48154660400051	25.90204566127668	47.31856231495082	n
37.67052745665409	34.94085546635435	46.62739222517906	o
37.61269897755950	24.80998291719779	54.35774070399691	h
44.19405247220149	35.04792981753192	46.82179597614527	c
45.32817587571405	36.81291952996737	47.57238592777115	n
45.03143548087583	28.93915784395313	50.83812572526863	c
46.17915727446935	29.39708680296724	52.64405606422172	o
40.40213163548835	27.33046568767947	50.23315520258629	c
38.73356538664263	26.64457998027404	51.52501146126263	n
44.15132750798086	25.03551369926916	48.01755237266124	c
45.91802385375551	36.36502788331597	42.16401330915242	h
39.60034478491567	36.84754294411501	28.32341736209930	h
41.45965762850873	28.23542817911285	40.40381696168321	h
45.98869994887134	29.50177934321374	40.90366012755791	h
39.43364826397773	37.96733417455021	30.05755288659154	c
36.14871719187347	37.74008401419551	31.16847685979958	s
44.79618419231959	43.04896550200808	47.48043686467859	h
44.15595101813859	37.44111347887999	39.48454236797606	h
46.77581371281202	44.90090940273454	45.48210046130484	h
46.43127951429141	39.53124107673341	45.68744016893206	h
44.01966208027793	36.58793992796789	41.36669447066068	c
42.53821424542219	33.49011336377225	41.46016695495296	s

Table 34: Coordinates of **4** with full Lys358 Ser323 Glu 361 in bohr.

39.94924701039030	39.94417627883237	29.65226964451481	h
50.19277964349697	38.71473417560934	52.88793266007645	h
50.27120875024651	40.64098536572883	52.02651198523608	c
51.73385677099154	42.27181901159830	52.76161544785858	o
40.75590275376379	37.20875041819932	31.46247764311113	h
24.85492524131635	24.61341687472085	45.52866086647165	h
24.90831713364304	20.22819390754747	47.36216895617212	h
48.56289633325230	40.96601825922772	50.21804408361721	n
48.72352305387675	43.22235125247008	48.64201249537256	c
48.23030087846302	44.90998694923750	49.76502589059358	h
40.17060991594136	25.23693911116933	41.65756052456575	h
46.93427038290969	42.95054730702358	46.38030127630937	c
47.59972253237478	40.90661353489330	44.78102583473527	o
20.64303166912721	22.49898953141177	46.68227502563289	h
39.23761225206564	18.94578987036000	43.51119175217512	h
45.80939384283276	28.96363243801628	40.98803174889045	h
24.98881238780070	25.91948748398769	48.56049974467597	h
41.12115485302754	19.35133084155105	44.27107596826239	c
43.54120121236189	19.21895749816607	41.78383715540095	s
41.49395081983173	28.06465898966612	40.41045523486257	h
36.36362883221879	23.76294395026884	37.77440260471624	h
26.64514471889627	29.85623324675481	46.68344107246919	h
47.03194292261343	44.69532355496197	45.24351964770290	h
37.43618890929004	24.30808246740923	36.08856184704014	c
35.56052699867394	26.50283010388586	34.14939904524327	s
36.21147617266212	15.88246577605643	51.39412551210340	h
37.33225397241539	17.59955472368199	51.10243591011421	c
38.00817208207712	18.37222715109409	52.90125001354271	h
32.00182587680171	37.13374969253978	45.42641205524481	h
35.95166949858130	19.69827169227743	49.65244652477995	c
34.11243657945888	20.94606686733727	51.14280855941463	o
34.51427781321816	37.52357956012416	43.22678982823236	h
40.54354142820216	21.97183915644452	56.13537344491939	h
38.98387460565979	22.68858717828973	57.35364993159300	c
38.83269651566030	22.33331866679093	59.63832881671026	o
44.96782897978484	42.76267752836319	47.07222036139165	h
43.76701671750573	21.76114463688511	41.36871461223498	h
28.44930377476098	32.78846782199553	50.34916083509913	h
37.24532657066569	24.02840300091018	56.12721767647217	n
35.77212009433857	24.71263225594500	57.14333460426344	h
41.58643259399869	17.93048877587512	45.70628393791183	h
41.12121317610923	21.20878700913248	45.19307954576672	h
37.86240926095834	22.60540932541273	34.97561209434847	h

39.21976666502103	25.18502775435845	36.68075567859426	h
32.37589640033583	20.50423895426035	50.48631376008440	h
37.40292615895782	24.48458406810161	54.23313532453248	h
39.02305498510812	17.02524821730764	50.01733293175842	h
32.46399196427624	24.51777413912992	47.61955119726301	h
31.89354856095402	39.64563479270676	43.16925981272813	h
35.18660861423166	25.38218292964820	49.31722635815172	h
47.83561973473216	26.74122108434207	42.57051626465526	h
32.46809892668190	37.67978452786387	43.47739099576508	c
30.78613002442007	35.60261206615176	41.25415087128184	s
26.09029273790488	32.69882575600892	45.04076325200661	h
26.32837874657772	31.89722258538349	46.93558980450335	c
24.59911319748768	32.06184983731730	48.06348994422720	h
46.90757349012490	39.33206470143235	45.55133131360611	h
28.59448687849555	33.11762265526345	48.29167169813438	c
31.15405151973110	32.11336381979844	47.35865655991602	c
31.66241165898214	29.40448094052968	48.25152207422732	c
33.87843267752407	28.23865760127386	46.84395197785983	c
34.25219201676307	25.52561761065475	47.58233148587923	n
20.48968978389725	25.83065999636581	46.78647864024759	h
21.36784766846955	24.18147081703466	47.68014189775082	c
20.77017676816403	24.00352779893370	49.65517254659523	h
47.56410325579927	39.42815478751634	49.54694098751646	h
24.26535228547571	24.28585827390634	47.49515648638210	c
25.53082115840004	21.87979605698871	48.47520998278112	c
28.45297614871093	21.86167131911518	48.46110295505365	c
29.55577331284979	23.72562496072914	47.42428104994153	o
29.48515377264194	19.97151033464982	49.49352537057744	o
28.52163376164510	35.18229168774020	48.02297634085220	h
39.59844470309151	36.85092065948808	28.32606486840042	h
32.69632392685106	33.35405652096636	48.00362596339588	h
31.19329844036844	32.20588741756346	45.27446420380922	h
39.43173969728328	37.97080235111289	30.06033550831059	c
36.15698321966816	37.80726867175910	31.20184951441298	s
24.93932707571551	21.47988474959299	50.43406355086815	h
44.15935921479406	37.44400126385790	39.48758949466083	h
29.99131562541332	28.20536413894000	47.94715393418107	h
32.04528233658225	29.38774676217173	50.30282756236201	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.78311189298088	33.36645679256819	41.35863023232537	s
44.02125967159002	25.74102325871928	42.42035859844506	n
45.98489593330139	29.64354566108853	45.51484307393709	s
35.09791843168621	18.92819469593860	47.90302098998554	h
40.16296857287750	28.51122092489965	44.77011883311631	s
39.57981292889075	33.95426633238633	45.81518669762991	c
37.74924209485291	35.15008943199760	45.97876069669510	o

44.38219565304914	34.94688326246779	46.74481086667152	c
45.57896209673292	36.70000509447659	47.42350171686547	n
41.87046665241328	31.44780261594938	49.37014692392275	c
41.26588604119951	32.60713155781399	51.16295985124339	o
40.12863497064694	26.80854006633245	49.95585666782794	c
38.39912236544585	25.89569785424638	51.02019044259372	n
45.02628269922369	27.82202425230216	50.60806833814257	c
46.47945330689575	27.47872811876032	52.22345159871097	o
45.97075454164143	27.65288405087058	42.59517027245959	c
41.51680684884951	26.77128574107006	42.03847404850777	c
42.37437485864142	32.18403668357021	45.59528682720281	fe
42.86179181191825	28.18722213084330	48.13813120172235	fe
37.02680618581400	37.16928455500219	38.47419705212264	s
39.81376399766702	32.33460380709442	34.76204866158224	s
32.94603168595165	32.98784005823957	35.00991316525585	s
36.27827840622816	30.54790335080099	40.25474859821301	s
36.15843730422294	30.22952412201798	36.07974128566188	fe
33.92872342323863	34.03366771330903	38.90531953574860	fe
39.24575223209831	33.45166644653187	38.76789897317737	fe
36.62961776379770	35.37074191507998	34.67299254488744	fe
35.65480856550457	29.23950213169443	47.21722698576540	h
33.56431598759734	28.30020219121526	44.79285487750884	h
42.79971299307896	37.78640950880764	42.53583455383985	h
45.90647105798671	36.53821045537510	42.22179811727421	h
37.39254937052731	21.10534073817756	49.07889544652819	h
50.68292848113515	43.46691418523635	47.97944368681893	h
43.37401038920866	25.36476837279334	47.79226535719732	h
44.00905656623939	24.79700770355340	44.12801793900174	h
35.45279223797677	24.67107435203379	46.32501634932026	h

Table 35: Coordinates of μ -H with full Glu362 Lys358 Ser323 in bohr.

39.95737936604244	39.94272242777944	29.65524971607617	h
50.19002015137168	38.71614357283621	52.89154397199607	h
50.27120875024651	40.64098536572883	52.02651198523608	c
51.73385677099154	42.27181901159830	52.76161544785858	o
40.74579435687647	37.20192669689972	31.46809917872051	h
24.86548116721314	24.61156548710262	45.53933800724472	h
24.97159244648610	20.26302331458172	47.46750118051183	h
48.56289633325230	40.96601825922772	50.21804408361721	n
48.72352305387675	43.22235125247008	48.64201249537256	c
48.33675481914553	44.91833308983004	49.79161580962818	h
40.62980268100653	25.16316135326368	41.45662517841801	h
46.81246285636229	42.99465100958617	46.47328338809911	c
47.31643889855133	40.90587586930994	44.87671354868815	o
20.65831044419004	22.49414462006352	46.68064603721596	h
39.23761225206564	18.94578987036000	43.51119175217512	h
46.06076456776020	29.41932658756284	41.00818810163459	h
24.96295533374497	25.97869177415585	48.54488281839785	h
41.12115485302754	19.35133084155105	44.27107596826239	c
43.57769211997417	19.11201590602567	41.85161621969758	s
41.60701155645909	28.18575042017789	40.34307748446647	h
36.36362883221879	23.76294395026884	37.77440260471624	h
26.65600726116071	29.85738881650184	46.68703475646849	h
46.91817342553789	44.72063331825941	45.30768572071749	h
37.43618890929004	24.30808246740923	36.08856184704014	c
35.54862516156948	26.48055065080534	34.13654720696614	s
36.21147617266212	15.88246577605643	51.39412551210340	h
37.33225397241539	17.59955472368199	51.10243591011421	c
38.00817208207712	18.37222715109409	52.90125001354271	h
31.99544445316287	37.13595612722620	45.42517814899755	h
35.97816061347027	19.70860283503808	49.63525255622503	c
34.21349011888157	21.05201996463652	51.12778481589238	o
34.51587904657948	37.51552227866374	43.23361693827239	h
40.54228211150776	21.96657248558305	56.13615107061623	h
38.98387460565979	22.68858717828973	57.35364993159300	c
38.83269651566030	22.33331866679093	59.63832881671026	o
44.87925410432636	42.89345968749473	47.26923553930067	h
43.02013096931515	21.26099428540273	40.57949157747937	h
28.46687062784310	32.78627867400764	50.34080928640501	h
37.24532657066569	24.02840300091018	56.12721767647217	n
35.78306567256976	24.72909103498235	57.14852818003477	h
41.58622280830427	17.94712112712446	45.72154234352105	h
41.14534669055193	21.21670844760489	45.17001590302583	h
37.88001822948241	22.60287631857866	34.98452640067629	h

39.21046690910044	25.20542012420540	36.68111835237374	h
32.44332165065944	20.63357710066679	50.53476270993265	h
37.40763784684177	24.53702674401267	54.25267385032226	h
39.02645236543259	17.01287360506790	50.02908301928827	h
32.54888341359948	24.59492202967842	47.59706102349741	h
31.89354856095402	39.64563479270676	43.16925981272813	h
35.23058560203042	25.55876656318119	49.28032045776786	h
48.16173119783321	27.15784001513141	42.44414408433926	h
32.46809892668190	37.67978452786387	43.47739099576508	c
30.78319759997941	35.60758213746922	41.25100702172251	s
26.09029273790488	32.69882575600892	45.04076325200661	h
26.32837874657772	31.89722258538349	46.93558980450335	c
24.59911319748768	32.06184983731730	48.06348994422720	h
46.57259731928436	39.36315946658286	45.67196034736729	h
28.59012236875703	33.13491047686573	48.28461850367237	c
31.15466373733133	32.17633789438874	47.31743568075196	c
31.72810713546570	29.48261302789832	48.21243409054317	c
33.88971619375422	28.31204354282311	46.72529066059634	c
34.31745938828898	25.62467013058772	47.53319842167686	n
20.48968978389725	25.83065999636581	46.78647864024759	h
21.36784766846955	24.18147081703466	47.68014189775082	c
20.77017676816403	24.00352779893370	49.65517254659523	h
47.53839322587545	39.43716446098076	49.56493688582658	h
24.26971299586146	24.31344632919262	47.50860551531394	c
25.56900764400129	21.94774107610228	48.54436947783627	c
28.49532280030526	21.95910136262592	48.53881033388767	c
29.59442661183418	23.78584223573279	47.43797890659254	o
29.53502651236058	20.11299517586380	49.64654371144531	o
28.48545626150309	35.20072577682629	48.03408549338342	h
39.59844470309151	36.85092065948808	28.32606486840042	h
32.68613600239106	33.44398359571001	47.92998451535406	h
31.16060743292188	32.26221273860217	45.23280386945756	h
39.43173969728328	37.97080235111289	30.06033550831059	c
36.15134788714438	37.81911835626078	31.19045642912791	s
24.97833386247566	21.58329105544128	50.51041770682028	h
44.15935921479406	37.44400126385790	39.48758949466083	h
30.05605966526330	28.26492899137047	47.99484621326150	h
32.20403664852789	29.49142586025016	50.24443112165523	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.72440700865703	33.39560686869410	41.35159989386337	s
44.43797521759721	25.99136065226755	42.03286976274615	n
46.08227479916858	29.80372092812541	45.52133233920505	s
35.06717720897112	18.92756251570634	47.92012238806102	h
40.41514796240077	28.31642024072904	44.72703990039344	s
39.47740667390519	33.64979891056170	46.03757392974864	c
37.57713610096977	34.68574329083155	46.44558454644424	o

44.15755576580603	34.92918202440074	46.81924311097406	c
45.28622425617752	36.71133337291813	47.55415614689357	n
42.15669626395312	31.14614575263614	48.45157190349255	h
44.85509430205089	22.78593558070867	48.05122955538672	o
40.17072557247688	27.09841577414771	50.02581129058582	c
38.36391096415483	26.38823303782039	51.11227139768440	n
44.81721818108562	28.76043333648836	50.90321447039906	c
45.91385740872249	29.21666710090226	52.74660085466407	o
46.25139643193322	27.96668932695540	42.48633034585760	c
41.84495850265404	26.79553642459558	41.87230895620519	c
42.34084994342941	32.12112214833284	45.50903346627519	fe
43.09828912883406	28.00509870094916	48.14219303438867	fe
36.97939439249861	37.16209312172279	38.44606069644885	s
39.79081067467681	32.33835506935928	34.73261618432159	s
32.91389252556160	32.95225445834484	35.01055395382107	s
36.29996390266501	30.52708520560754	40.25100991430285	s
33.91310319256615	34.00402509683678	38.90513151382503	fe
36.14940369240595	30.21519171741562	36.06942833877219	fe
36.58411480913765	35.35316726596446	34.65436977384031	fe
39.22853531208595	33.46283320597925	38.74518329933359	fe
35.67102628786680	29.34057965552529	46.98242474309786	h
33.47385891167676	28.30251470795948	44.69198753509311	h
42.82964858405723	37.80328921316709	42.54948639003411	h
45.90878388632184	36.50100132660081	42.21788002801442	h
37.44989636488373	21.05487678136455	48.99156856453384	h
50.65433083174727	43.40663306864526	47.88165984447469	h
44.12140494795389	24.86746442630670	48.02434569902817	c
44.63611356547961	24.58168253486269	43.34044118283535	h
35.54298811511392	24.76401336787865	46.30328893280543	h

Table 36: Coordinates of **4** with unconstrained Lys358 in bohr.

39.94970995320045	39.94449140770534	29.65034084188372	h
50.19141644760933	38.71783618325333	52.88751070036864	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.76481132189645	37.21123884125993	31.46005916496632	h
37.16946017728381	20.89663079427748	48.79815916894791	h
32.45523510010127	20.85477156309295	50.85742198553563	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.20903896739147	44.91212697811972	49.76322579121684	h
47.72282269147276	26.66829404131839	42.49093743041706	h
46.94859948030426	42.94690376586959	46.36993304484538	c
47.63981077122377	40.91300809508022	44.76974472063345	o
36.27607531423431	30.55110933442581	40.26447441647528	s
39.24256703837632	18.94525451094879	43.51072978972661	h
45.87600669183531	27.61447251443999	42.55186517392296	c
41.39411766446459	26.80390794384908	42.09075382471008	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.53877384122561	19.26221535472120	41.77355630132161	s
42.41894874283816	32.20181253051467	45.61989978756171	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
42.90670496687653	28.19576124740956	48.15053180310419	fe
37.04331552160291	37.17351137023062	38.48680079788210	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.56576740982435	26.50451845624533	34.14941319896872	s
39.25336871571113	33.44702888955072	38.78320907912227	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
36.16568652657562	30.23174061807603	36.08942263037529	fe
33.93860552302731	34.04239762427533	38.90881502890547	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.25958916882007	21.04752155309255	51.43780110520726	o
42.80133551984112	37.78815791974147	42.53584159643988	h
40.55468678984897	21.98376380386268	56.13650749617879	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
43.89674096621341	24.80738707988000	44.14530716863236	h
47.57282181708613	39.42624871007396	49.54142321741629	h
50.68284405581706	43.48154011851089	47.99669268111690	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.74498966613787	24.66178730531271	57.12749477487069	h
36.64749834091163	35.37268154543327	34.68311911101261	fe
41.11749803116230	21.19669471034995	45.21484204686914	h
41.60752083098122	17.91471253489303	45.68542705850156	h
43.70624967987892	21.81241141475812	41.35913803776221	h

39.82289649742346	32.33192794193292	34.77608897065797	s
32.95735123961297	32.99621242862903	35.01348986341586	s
46.55683213108801	27.46141768534372	52.20320905438720	o
39.22363148969489	25.18511106246557	36.68271332473530	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.86923011378261	22.60535815104888	34.97495471521325	h
34.51999171808411	37.53124398444847	43.22478471820337	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.80236749015335	35.56951488447131	41.27790143534875	s
32.01566530936486	37.14366993265054	45.43212528289605	h
32.91059396748889	29.23483708261949	46.04267579849650	h
35.73203898007876	29.56229391191362	47.87397743186790	h
32.25242539328359	24.99506096508487	48.11617411462774	h
35.32366258190019	25.39626420627196	49.41821707503506	h
34.98852684218903	25.26238371768829	46.31874418245774	h
32.72295632071594	29.31064395355455	49.42405177985837	h
33.85459117497993	28.69638448490366	47.80400065405499	c
34.11255986078346	25.89500655907372	47.92758221117468	n
34.64140114840309	18.70767642685754	48.27224208267379	h
37.38012500694078	24.41835857789339	54.21839176126475	h
25.31074997276070	20.45050122646074	46.87974848248626	h
24.68853900806434	21.15484743824525	50.09030140850370	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.42557147992124	22.24567277648630	48.80599909999065	c
29.38170303086645	24.34510937479531	48.13109988256409	o
29.56246509966879	20.38968809181083	49.78665373918476	o
45.90818032104542	36.54306844702569	42.21860354584277	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.36227294887104	28.09644807620262	40.46275893545671	h
45.70309445265132	28.92313630773264	40.94460535609559	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.16377003091291	37.79933539340567	31.20744162077009	s
44.97892076357295	42.74302476880855	47.04820192260591	h
44.15935921479406	37.44400126385790	39.48758947576357	h
47.03985825225678	44.69498797866856	45.23711245300796	h
46.97115295327998	39.32895314877015	45.54097905143214	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.78956428520479	33.36522296794841	41.37434454347341	s
43.88900940590787	25.73753442998046	42.42940675603520	n
45.99148458424715	29.61364938759427	45.46523457119257	s
40.01914399234398	25.28904181450209	41.73782420491604	h
40.11872743580089	28.57096936574424	44.84810366509569	s
39.68159485991787	34.05288032043654	45.86943310609302	c
37.90431034155634	35.32461824986427	46.04684440399144	o
44.47151667646590	34.93412827326256	46.75509596893068	c

45.67798340174768	36.68274785593689	47.42956003809530	n
41.91984281395808	31.44283044755417	49.40538318194676	c
41.31486402593818	32.60057282065029	51.19970438833793	o
40.21404059426785	26.76171372148910	49.97454323958098	c
38.50064892865817	25.79619697191233	51.01686732073927	n
45.09795106468607	27.81637528867618	50.59517253498615	c
43.41287994907074	25.37806051459727	47.76520782402423	h

Table 37: Coordinates of **TS(4, μ -H)** with unconstrained Lys358 in bohr.

39.98630106063008	39.93580287409141	29.65752384631430	h
50.18973718975013	38.71709022949315	52.88653379494414	h
50.26629540562974	40.64463389775288	52.02813809456664	c
51.72891508048290	42.27543730800434	52.76322643938014	o
40.73751318895246	37.18748625191881	31.47150209598838	h
37.17249784550082	20.85445216466725	48.75205745869332	h
32.48611227512792	20.90910585982162	50.89800647219408	h
48.55801700370579	40.96966112207340	50.21970420801802	n
48.71863994487799	43.22595065161487	48.64370285539137	c
48.22069083034796	44.91443372623274	49.76328903192549	h
47.83215966887920	26.55736213616034	42.54326243271883	h
46.92520189471198	42.93025441031744	46.38546706295719	c
47.58530649366564	40.86417895480076	44.81555893848993	o
36.26989957893611	30.54788306470442	40.18669489296673	s
39.24180893694676	18.94488801746411	43.50988956079966	h
46.00521046412705	27.54150792594105	42.52331961677231	c
41.53090325135286	26.76345704035042	41.81864694411662	c
41.12531597326299	19.35042135416161	44.26975977401633	c
43.55534345106957	19.08507360751367	41.80569589674919	s
42.48625494818008	32.16458727296136	45.41827102357949	fe
36.36788132071239	23.76194919843665	37.77321205836024	h
42.81792158556659	27.91756581418650	47.94631052472169	fe
37.00749969426204	37.18327914283385	38.42718776515677	s
37.44042183911824	24.30707849371355	36.08740438978858	c
35.56746697471249	26.48577351213139	34.12589775510695	s
39.23312326934840	33.46933709286006	38.72279489511698	fe
36.89250708753310	18.18380460007519	50.71378822120659	h
36.16040603773449	30.24718656001455	36.01759871948589	fe
33.92472979898139	34.04310112586005	38.86137759511772	fe
35.78505387896799	19.64332323435724	49.74796998570974	c
34.30429098559765	21.10995543677989	51.42873404675513	o
42.79321346522004	37.77131105124435	42.54378734647526	h
40.55663373250982	21.98943158126685	56.13533966869186	h
38.98807729987000	22.68761344021204	57.35208051404620	c
38.83690109959663	22.33235248761774	59.63671593546258	o
43.93219739396003	24.66024648449633	43.89444008729319	h
47.57026006155520	39.42307338415046	49.54524007977357	h
50.67721136416674	43.47122728674772	47.97889728868997	h
37.24956327994614	24.02740469639287	56.12567282536499	n
35.72333144632334	24.62351183762326	57.11815416043933	h
36.61033439782793	35.38825038074236	34.62618180380881	fe
41.15440287081451	21.23707386660562	45.12900176050402	h
41.57338917128853	17.97593116569616	45.75399607745697	h

43.71069517590818	21.58478898048334	41.19341021902071	h
39.81080532106653	32.35911907078925	34.70760811007164	s
32.92848921934118	32.99631565245878	34.96250983187416	s
45.66291934712414	23.22621008312284	48.77307990547803	o
39.21901528589068	25.19395924907271	36.67926423510474	h
31.89788723985617	39.64433382965327	43.16796440546944	h
37.87937545817660	22.59958675084705	34.98562977376181	h
34.52263690354593	37.52945976762889	43.23158144822708	h
32.47242634281635	37.67852166168906	43.47608991932802	c
30.80830199038994	35.56290582960024	41.27566873786557	s
32.00966213514486	37.14449431380852	45.43071283822026	h
33.15919738452059	29.09525107030412	45.91409191956490	h
35.83148834023589	29.36404346619468	47.94350863935992	h
32.15139388582081	24.89072417742537	47.97294132291605	h
35.13308311828884	25.12902726568493	49.44605215958391	h
35.02570999389602	25.04034281723214	46.33096416603395	h
32.71582236204831	29.19313263730509	49.26941886073516	h
33.94752562640499	28.53353403823307	47.74315306832631	c
34.09036393282207	25.72271978616037	47.88467916940482	n
34.60097997460251	18.69991644853168	48.30854616836045	h
37.36749785081101	24.34357897751926	54.20456417027994	h
25.30943877190041	20.45655956709250	46.87256220388544	h
24.69803840829071	21.14892540666744	50.09058347366661	h
24.62543687453897	23.63635044126507	47.76473076342085	h
25.56849713831252	21.89019247916562	48.35720147758109	c
28.42234733420207	22.25680946011624	48.78252455981500	c
29.38215307268881	24.30215063715802	47.94516963301441	o
29.56299253376540	20.48101449299674	49.89080677571505	o
45.90341056486107	36.53071377589146	42.22588492517721	h
39.60263513297916	36.84967455518400	28.32505575464967	h
41.55121148729051	28.04233504167338	40.17832003856638	h
45.93253222503504	28.88250883625574	40.93409975600588	h
39.43593294286286	37.96953381575970	30.05929332435266	c
36.14824669498186	37.85029502056205	31.16688788434515	s
44.95979300560390	42.75572149353074	47.08466502983971	h
44.15850781758571	37.44327910501924	39.48682704686118	h
47.02298073271571	44.66007665727140	45.22523168245265	h
46.89182472610249	39.29123761245541	45.59734538133690	h
44.02220943109442	36.59006020068013	41.36908686393492	c
42.79021325680941	33.38187512504219	41.30173474949983	s
43.99909344718747	25.69924130700550	42.25046913428156	n
45.98241236344929	29.56502027713547	45.43905958030285	s
40.15046063680271	25.25527855726276	41.46936760847911	h
40.15590548159340	28.70396846062544	44.44413697921956	s
39.80644288844388	33.89825171254722	46.20679384905586	c
38.04070823350040	35.09617296456891	46.76863889729175	o

44.46610036576906	34.84860337547261	46.74271478988804	c
45.63561669766173	36.61287280162465	47.45844544076859	n
43.44996318541069	30.29328212026164	50.26049249757308	c
43.88145115114720	31.57729188399720	51.99483961591407	o
40.29298473177499	26.42686180095071	49.95892789372925	c
38.66550611771593	25.40959532732916	51.11126682639428	n
44.51526225023439	25.06967845295469	48.34884454893395	c
39.89223122187003	27.79276596482755	47.86261822944024	h

Table 38: Coordinates of $\mu\text{-H}$ with unconstrained Lys358 in bohr.

39.94536098515376	39.94558521901180	29.64984498884592	h
50.18589011145138	38.72046702786228	52.89368031176671	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.76591144325174	37.21257003658596	31.45972933492988	h
37.16600587060036	20.84907572577414	48.72982999876624	h
32.49913415073704	20.94482789053202	50.88788566950477	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
48.35319403473351	44.92259512378371	49.80146133670697	h
48.14933143331843	27.09061290653502	42.52801365381749	h
46.79401164370058	43.02404218301045	46.48854444781441	c
47.28351740495305	40.95681269882668	44.86099320517567	o
36.33433713015018	30.48893288604669	40.26429116680809	s
39.24256703837632	18.94525451094879	43.51072978972661	h
46.25094014533186	27.92817727694462	42.56368514613918	c
41.82581419369587	26.81020269310456	41.95870300131482	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.58278260216571	19.10624915430165	41.84909824924603	s
42.39558213439577	32.15725113203294	45.54436123161958	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.09500700886455	28.05046131131472	48.20891536149795	fe
37.03013719943346	37.13771564465441	38.48718758959130	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.55290179891590	26.47473013173392	34.13046359207358	s
36.62505991405988	35.34237993423749	34.68677969898672	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
36.17440702482594	30.20080268798576	36.07981025049916	fe
33.95685721726612	33.98483938233630	38.93536636572224	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.31930629625892	21.11114393739216	51.43257196521933	o
42.80603172513700	37.78993833631565	42.53876678804861	h
40.55206830878886	21.97482414212240	56.13749885745509	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
44.58318104405145	24.58998387187572	43.47434438696388	h
47.53939457933966	39.43811740389336	49.56145936788292	h
50.64595728071926	43.40261310066373	47.86969463353812	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.76349798443849	24.69056794819222	57.13730373072499	h
39.26743390870327	33.42572272075060	38.76737673231036	fe
41.15199286848640	21.21833658136948	45.16415444037001	h
41.59128780826535	17.95115560070711	45.72580653096558	h
43.12442856888329	21.32813684017909	40.66296809980936	h

39.81942130769003	32.31911557320215	34.74820765192623	s
32.94559258727087	32.95216970921167	35.03948799816235	s
45.86777239306905	29.25167687296574	52.84230381958211	o
39.21130824367709	25.21056299130239	36.68474829716826	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.89340668217140	22.60164620881588	34.98813944219414	h
34.52243551419873	37.53196373527594	43.23384771320880	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.82005359829466	35.54569081275062	41.28960025120775	s
32.01535496948171	37.14910238471158	45.43379361778013	h
32.77674040854414	28.92497994009762	45.32648088883027	h
35.63811210393873	29.62380306092826	46.97029413319514	h
32.25232721167704	25.09390897610826	48.05539094775021	h
35.27029828314377	25.80534938655108	49.34070437492191	h
35.01620757186368	25.10612369933344	46.31358099694804	h
32.68257866672597	29.62505110424505	48.63678322119661	h
33.77840823719846	28.73246685074183	47.12637701703355	c
34.08892087787460	26.00100455183419	47.76057907706080	n
34.59565306419727	18.69390759116833	48.31763655753674	h
37.37205213761581	24.48161210508435	54.23889778399253	h
25.33961094524512	20.46072010331822	46.86521804619866	h
24.68080084366702	21.13746413321902	50.07824466908549	h
24.62591155484430	23.63680664004891	47.76565183483143	h
25.56899105602981	21.89061475736551	48.35813405742378	c
28.42469469294420	22.28247108160072	48.82763349754814	c
29.36917183562683	24.36651043718658	48.09477977899674	o
29.57168542392476	20.46910319316137	49.87762982377509	o
45.90599379369210	36.53517122094636	42.22708816527022	h
39.60339958388850	36.85038530007687	28.32560284926011	h
41.61048032333236	28.18355075528677	40.41122541633401	h
46.08068354925875	29.36521631470420	41.06848752480148	h
39.43669450249122	37.97026702949620	30.05987347027303	c
36.16541265158544	37.79439487979737	31.21545616577473	s
44.86635146487759	42.91579605661371	47.29773699671546	h
44.15935921479406	37.44400126385790	39.48758947576357	h
46.89265192554651	44.76412245849668	45.34298069406751	h
46.57459801510694	39.40004860988923	45.66083903224690	h
44.02305980785066	36.59076695825087	41.36988432835967	c
42.77546048390057	33.37759400830505	41.36976963304403	s
44.40797293802168	25.97241446125015	42.13510060326031	n
46.10794599024536	29.79701669670271	45.58008142603345	s
40.58936440589550	25.18926127072505	41.56217942900862	h
40.41465160779202	28.38397204091311	44.79374986011141	s
39.56167709342465	33.74263130428758	46.05955854609473	c
37.68544324956570	34.82346939957529	46.45904834968433	o
44.23411074940996	34.95570396416441	46.83572742820528	c

45.36140574377892	36.73921496851902	47.57002142321753	n
42.19284448371019	31.20198325757793	48.49496084450953	h
44.80875212658318	22.81652214624388	48.13989893523904	o
40.14368634251475	27.17643789876163	50.06180135620461	c
38.30873743426927	26.48410548188727	51.11144641258149	n
44.79457845967270	28.79896193696213	50.98402321430921	c
44.08964402945774	24.90351116268778	48.10586875696801	c

Table 39: Coordinates of \mathbf{O}^* in H_{ox} in bohr.

16.21794891631631	2.02289955745724	1.94709224735415	h
-4.99143826943683	15.40536870793692	-2.59744504314291	h
-3.23215543884491	16.39787546194912	-3.20801229787199	c
-3.14394113360409	18.68262426693300	-3.54127683837136	o
13.09724259689721	1.65201224569944	3.17478036875209	h
-9.56345018962812	-6.37717538653388	0.98894451577334	h
-10.46437412941617	-8.98523083394852	-3.30392802012061	h
-1.30865612854544	14.82782296716395	-3.56737017670527	n
1.21410179215526	15.88771743834136	-3.90270585703764	c
1.51868809972487	16.42998469909093	-5.89652712422306	h
-2.72134212760118	3.89643987792998	8.80964180908058	h
3.19564299414164	13.93506599094273	-3.08620156781322	c
3.01271692623487	13.30361145407838	-0.48693746005405	o
2.64265726286132	-3.17527905337057	-0.40575526049883	s
-6.78925306433472	-7.39737826971441	6.07024817857103	h
-2.04907430507398	3.16016440756612	6.98941349797289	c
-1.44646881615833	-0.80621948382980	4.74510942419362	c
-7.47977788766863	-5.54224736089107	6.67931068810872	c
-6.03770934602837	-4.57230077136612	9.66914820637675	s
-1.63165939292588	4.23914189617844	0.70184877862236	fe
1.03665650901836	-8.17808271345913	4.48400451034691	h
-6.50692059417794	2.58601437329417	2.29079195341485	fe
7.63030460671816	0.93445290570506	-2.64097478988511	s
2.53657937757890	-7.51797114238087	5.75040258328524	c
5.64409961445314	-8.07778944199015	4.30710228488114	s
5.01232753737566	0.30953089335618	0.74678203832774	fe
-12.67473327103450	-7.60383840777446	1.24211320250604	h
6.07605827843027	-3.13583115768586	-3.21095260981695	fe
5.92592476357918	-4.71851759555208	1.78222590829535	fe
-10.89099621521343	-7.80140927414254	0.20841600459942	c
-11.25374207050273	-7.46697351519885	-2.41637739806313	o
4.04150277084394	6.27701650469044	-1.58539925441402	h
-15.51174139525598	-1.03834808382337	-1.29026603234978	h
-15.85035755285023	-1.45558611421594	-3.32454603882197	c
-17.87683181915286	-1.15034999160247	-4.40558843506418	o
-4.25933186206027	0.01968084716537	7.23243306248361	h
-1.46046770665576	13.01655605271310	-2.84698092938876	h
1.38131024250892	17.61272530908431	-2.75260034567863	h
-13.82130192066086	-2.26651294787769	-4.56818425031088	n
-14.06622377440420	-2.88197612089748	-6.36660043300840	h
9.84919056971541	-1.56047770673322	-0.00711481561377	fe
-7.14080011903635	-4.13214602312710	5.19931686916926	h
-9.52060548837882	-5.63559631824832	7.01779176424289	h
-3.61398496453649	-4.49267506384146	8.85704135849832	h
7.59972325659380	-1.14179167200377	3.71321847737725	s
8.80019983554538	-5.611039311708946	-1.35450622667224	s
-9.81718092479626	0.30139304054145	6.06552807978654	o
2.25525991716090	-5.49832919663762	6.13274778382049	h
6.34206827411624	-0.29135986367764	-10.04097283775169	h
2.41990975557707	-8.56093194930770	7.54515176244529	h
4.61113095981279	0.45589284296561	-7.26720066088543	h
4.89153339783241	-0.98079809448967	-8.73333716131375	c
5.76489823824563	-4.01318639157285	-7.30949019483457	s
3.11392944508182	-1.19772952037963	-9.79147997433879	h
-4.71356595858340	-5.53824943994650	-3.50457765863613	h
-1.36851373146470	-5.04130205572433	-3.80931008918418	h
-5.50008462674974	-1.16891509120019	-3.85753666201219	h
-2.50417212045051	0.55544102601874	5.12726040288102	h

Table 41: Coordinates of $\mu\text{-H}^{\text{Lys*}}$ in H_{ox} in bohr.

16.10285912268195	1.75089359657741	1.86421005849613	h
-4.75418495709299	15.61820562167378	-2.58566941573371	h
-2.96528453602107	16.55828486406920	-3.19612403081966	c
-2.81781219895269	18.83673710160460	-3.55054972446671	o
12.96927644579657	1.32898576747393	3.04882329630475	h
-9.85076448452397	-6.02228675282315	1.29755836951557	h
-10.69380288400938	-8.25518463100301	-3.04229285255910	h
-1.09183462214205	14.93181270609622	-3.56840763634790	n
1.45458833882194	15.91744849946588	-3.94800448197986	c
1.55001969401685	16.94285884216488	-5.76093858926858	h
-1.80469081052286	4.51905943915153	8.61169311106675	h
3.34532858814878	13.72192655179647	-3.92068759142808	c
3.42833373355209	12.44946597258421	-1.56499884808812	o
2.65094613168874	-3.22227149143825	-0.36688901718870	s
-7.05613341578919	-7.04864632088196	6.33830016022300	h
-1.29616293732906	3.53904735056402	6.85414268702383	c
-1.27181108376041	-0.62825397781711	4.92987772265830	c
-7.68572590994880	-5.16983336426021	6.94063146530346	c
-5.91412615281471	-4.14030305460724	9.73463864148368	s
-1.56670128709976	3.89334113209440	0.37055736543768	fe
0.72148231671355	-8.06245226159690	4.65043269017510	h
-5.97087659638256	3.06953827166886	2.43438662949727	fe
7.70227608148439	0.63085686977093	-2.71293213135736	s
2.25702652273022	-7.43425816476978	5.89002877748264	c
5.34205575905952	-8.09642294009485	4.43876564797142	s
5.06909640737315	0.18541600212407	0.64474510206134	fe
-13.01260874327886	-7.12975903534506	1.59446586659397	h
5.96929399356778	-3.33258361911218	-3.23308745266845	fe
5.86184457813589	-4.85038131319483	1.82461733550821	fe
-11.24992701594246	-7.38606447940407	0.53788219558755	c
-11.72246015478443	-6.98371158375164	-2.06568671655985	o
4.01681538140875	6.49661315144786	-1.57695777400618	h
-15.67916529569682	-0.48077021906261	-0.96682161965606	h
-16.07887646396733	-0.93307873038133	-2.98117335328001	c
-18.11103880590619	-0.57999285255691	-4.03657405573218	o
-3.73433579760054	0.63807390788684	7.60231616096400	h
-1.30113102027830	13.08354207048794	-2.97060700162363	h
1.91302296410284	17.27578510277588	-2.43642583197882	h
-14.09115292158383	-1.81112107709836	-4.24570626653297	n
-14.37591704559320	-2.53106911253292	-5.99839941975885	h
9.86209772984678	-1.92536429157328	-0.06616231542521	fe
-7.48669767879599	-3.81320972986960	5.38646226330181	h
-9.67754874070817	-5.24934600735071	7.50189388953287	h
-3.57638517531923	-4.32760175294241	8.71660310082801	h
7.64602146023831	-1.28115500251950	3.62014477851176	s
8.60362509240888	-5.90315201975598	-1.37727931859385	s
-8.72904577009267	1.40353277230607	6.89316557169734	o
2.04167529274866	-5.40354082963399	6.25034816025330	h
6.03990673590814	-0.44992300337360	-10.01500044188978	h
2.13625286321975	-8.45453808677271	7.69638129603713	h
4.34214903475836	0.34753257933933	-7.21047303792366	h
4.58927170413968	-1.08731250752494	-8.68138670041155	c
5.43899146595212	-4.13997045934581	-7.28004706174084	s
2.78799567505040	-1.29141923088540	-9.69471434129163	h
-4.46315160219771	-5.82729303508756	-3.19783599899224	h
-1.53914122831459	-4.30003627521939	-3.84242091815978	h
-6.57051510632525	-1.99596541308222	-3.14422272809352	h

Table 43: Coordinates of O^* in H_{red} in bohr.

16.19761089875454	2.07010735462891	1.99801620089332	h
-4.99104372119488	15.40255647490740	-2.60302808304648	h
-3.23215543884491	16.39787546194912	-3.20801229787199	c
-3.14394113360409	18.68262426693300	-3.54127683837136	o
13.07017128378454	1.60681573416840	3.17688852270858	h
-9.60876223121320	-6.28481976251921	0.87767184288557	h
-10.50852836122751	-9.14146354947972	-3.25936009088745	h
-1.30865612854544	14.82782296716395	-3.56737017670527	n
1.21410179215526	15.88771743834136	-3.90270585703764	c
1.49576194281542	16.50207190608537	-5.88116374105230	h
-3.27445612828444	3.81486336444427	8.51767965473175	h
3.18485173169332	13.88444937510734	-3.17580354450744	c
2.97459540388835	13.13513206275528	-0.61870926871400	o
2.65104032170314	-3.25671919364799	-0.35706277651483	s
-6.78925306433472	-7.39737826971441	6.07024817857103	h
-2.50402449895483	3.05756133692353	6.74276513320774	c
-1.97402252073641	-0.87266637389850	4.44324319523037	c
-7.47977788766863	-5.54224736089107	6.67931068810872	c
-6.01110332594406	-4.65250276740715	9.70891390215729	s
-1.60301660502810	4.19626238532067	0.35441336243086	fe
1.03665650901836	-8.17808271345913	4.48400451034691	h
-6.60683655786973	2.82181853573194	1.78320102917198	fe
7.61239252411045	0.90692287174629	-2.69655915444970	s
2.53657937757890	-7.51797114238087	5.75040258328524	c
5.66187338442070	-8.10526776025119	4.35022636767485	s
9.83217465386266	-1.54104794489518	-0.06391426626938	fe
-12.67473327103450	-7.60383840777446	1.24211320250604	h
6.05413576399001	-3.18976159544114	-3.20811005898805	fe
4.98590897452024	0.28470986257185	0.72711805465791	fe
-10.89099621521343	-7.80140927414254	0.20841600459942	c
-11.34083562119876	-7.63057353353946	-2.41654977262925	o
4.03761931518250	6.19517989160264	-1.58204156720457	h
-15.51096009290613	-1.05286534676486	-1.28886747752777	h
-15.85035755285023	-1.45558611421594	-3.32454603882197	c
-17.87683181915286	-1.15034999160247	-4.40558843506418	o
-5.09345850311234	0.33066036993512	6.24431808452173	h
-1.46065784789140	12.98175429077087	-2.88272078074643	h
1.41147354807448	17.57018212917422	-2.69253171061628	h
-13.82130192066086	-2.26651294787769	-4.56818425031088	n
-14.00951939896348	-2.71937257101357	-6.41900329400708	h
5.96564798485951	-4.71623025257431	1.79440098781574	fe
-7.04906451327682	-4.12675497525280	5.22973757271566	h
-9.53625086956383	-5.59977379637750	6.91880238443558	h
-4.47596683907834	-2.75520616095018	8.84350791252955	h
7.64313998703295	-1.09067110909561	3.71594643329249	s
8.84596525416210	-5.639891282455313	-1.35662703997472	s
-10.37701512506696	1.08545297715893	5.44469180515985	o
2.25354786529993	-5.49278348527235	6.09756940565736	h
6.34206827411624	-0.29135986367764	-10.04097283775169	h
2.38390739806309	-8.52893949202293	7.56254644846875	h
4.62831475703493	0.43881054289094	-7.24785913690113	h
4.89153339783241	-0.98079809448967	-8.73333716131375	c
5.74922536352098	-4.03964806011918	-7.35206690062233	s
3.10317350397954	-1.15896115000196	-9.78286843785222	h
-4.67477616970243	-5.55975822265581	-3.47303729418692	h
-1.34250893123756	-4.94856197759879	-3.80429471120056	h
-5.61120083051292	-1.21311219008773	-4.06312312645565	h
-2.61488640381570	0.55140241488640	5.19047508422101	h

Table 45: Coordinates of $\mu\text{-H}^{\text{Lys*}}$ in H_{red} in bohr.

16.08639420351073	1.79554065719972	1.91885374306683	h
-4.74867964543885	15.61805050637601	-2.57222930820080	h
-2.96528453602107	16.55828486406920	-3.19612403081966	c
-2.81781219895269	18.83673710160460	-3.55054972446671	o
12.94878712989724	1.28938876102309	3.05931910725996	h
-9.84670641703596	-6.02288381685888	1.28686791444575	h
-10.86764527465978	-8.33962563705069	-3.08443600488087	h
-1.09183462214205	14.93181270609622	-3.56840763634790	n
1.45458833882194	15.91744849946588	-3.94800448197986	c
1.63784380008979	16.72494634385885	-5.86544225430699	h
-1.89172635574318	4.56447669503824	8.79369914041522	h
3.36413020237499	13.76921959264528	-3.55712919416398	c
3.29331956930086	12.78607627230891	-1.07302396859963	o
2.57911443135608	-3.26721127901543	-0.29410041378960	s
-7.05613341578919	-7.04864632088196	6.33830016022300	h
-1.43001492352965	3.61019043869930	7.00704316146985	c
-1.47656350893247	-0.51860414443833	4.99992906954741	c
-7.68572590994880	-5.16983336426021	6.94063146530346	c
-6.11926835398210	-4.22043222361712	9.88107612587523	s
-1.64864810155864	4.11438304467975	0.54052189002803	fe
0.72148231671355	-8.06245226159690	4.65043269017510	h
-6.09695073883102	3.29065759301006	2.54129213684481	fe
7.64816720529600	0.66063208821980	-2.79758558666770	s
2.25702652273022	-7.43425816476978	5.89002877748264	c
5.35628484909577	-8.11838617359072	4.47319650365726	s
5.83745332651925	-4.82291250954938	1.81182699459047	fe
-13.01260874327886	-7.12975903534506	1.59446586659397	h
5.90642648329766	-3.38233731682317	-3.22015732228906	fe
5.05199237125907	0.19030759544845	0.66863523072299	fe
-11.24992701594246	-7.38606447940407	0.53788219558755	c
-11.74464191744872	-6.97876942902102	-2.06115460991087	o
4.03465344493418	6.31844178897549	-1.58717019591098	h
-15.67257829977124	-0.47277233276017	-0.97099949718164	h
-16.07887646396733	-0.93307873038133	-2.98117335328001	c
-18.11103880590619	-0.57999285255691	-4.03657405573218	o
-3.97463196392449	0.79224881970011	7.60614914193874	h
-1.29152633633140	13.08398561063297	-2.92824289439903	h
1.81008290234458	17.45280845659285	-2.58632350613494	h
-14.09115292158383	-1.81112107709836	-4.24570626653297	n
-14.36000199618804	-2.53130790958415	-5.99995614896167	h
9.80646618427170	-1.84363155497355	-0.16765757772886	fe
-7.34878139325438	-3.77929300744781	5.44122661731728	h
-9.71730353520247	-5.21402742218510	7.34437795400064	h
-3.76463881178133	-3.93743020771626	8.92381406257722	h
7.69738746856743	-1.23698042805914	3.64217656610884	s
8.63959398031455	-5.91456371304779	-1.36931608418961	s
-8.89621926696289	1.54634192680124	6.94674356905794	o
2.04136380677228	-5.39668948278087	6.21647828922308	h
6.03990673590814	-0.44992300337360	-10.01500044188978	h
2.10118515040937	-8.42304519512115	7.71496866904745	h
4.39191959248381	0.32536800978546	-7.18061748575262	h
4.58927170413968	-1.08731250752494	-8.68138670041155	c
5.43027192686512	-4.17841507105795	-7.34560073613136	s
2.77263424475148	-1.23377334579856	-9.68117303848070	h
-4.52344349722016	-5.79428084411764	-3.20107892977227	h
-1.54704861389053	-4.36615357138489	-3.81977628476353	h
-6.52534007839687	-1.86313313157326	-3.31737792013765	h

Table 47: Coordinates of **0** without Lys358 in bohr.

39.98893223233126	39.93676446520319	29.64894702574521	h
50.20263162407044	38.71184312489439	52.87208279934966	h
50.26726579889218	40.64541851203997	52.02914170921436	c
51.72991381963722	42.27625215790944	52.76424517183686	o
40.75934668834746	37.19247015699189	31.45648011858079	h
37.09486014927054	20.74273035983896	48.54801535450148	h
32.75728442275260	21.42340150049197	51.12196068906989	h
48.55895338189797	40.97045140553887	50.22067380759550	n
48.71958010252243	43.22678439878122	48.64464221935084	c
47.90034243233574	44.86897470473526	49.64627702385295	h
47.42927774844706	26.51307021572314	42.71220092979515	h
47.32927595565944	42.79888485935179	46.13995442298319	c
48.45198155193744	40.86894166896477	44.66302513218010	o
36.37627989245117	30.55645383513205	40.23656433296561	s
39.24256703837632	18.94525451094879	43.51072978972661	h
45.63413798005277	27.53537753814214	42.93168834695108	c
41.09932618594128	26.78396576079727	43.17795001292839	c
41.12610965823549	19.35079551993436	44.27061393022483	c
43.42032501212206	19.68802776725886	41.67668997990456	s
42.73835832116895	32.55372209029871	45.81247267987251	fe
36.36858371301579	23.76240864754941	37.77394062337047	h
43.36272104544582	28.86019075043710	48.70855170465741	fe
37.14879066172823	37.18142389233551	38.51063315647952	s
37.44114371449799	24.30754714579254	36.08809980900259	c
35.61770280594568	26.53109543369609	34.13121557242849	s
39.34203407505009	33.42991295607325	38.81727015468763	fe
36.89321881508356	18.18415599464813	50.71476704264756	h
34.03528069688846	34.05926040768642	38.90760303777643	fe
36.27799467696826	30.26015703853829	36.06991396386021	fe
35.78574362900361	19.64370306930837	49.74892996658124	c
34.59581525371008	21.20608823008605	51.59569686002715	o
42.77753887334602	37.78563981799325	42.51619673992971	h
40.56047695607726	21.99206506708550	56.14209659092599	h
38.98882941086774	22.68805185667304	57.35318789355545	c
38.83765132086825	22.33278334517424	59.63786677867270	o
43.84793040524188	24.86188346337275	45.02375471399147	h
47.63138815123460	39.39768391116041	49.47619271748189	h
50.72366110808728	43.66409248057527	48.28372599903170	h
37.25028137587364	24.02786767929349	56.12675563843461	n
35.65450236276154	24.44219059005993	57.11341703642525	h
36.75313097767159	35.40078610791055	34.70395603988915	fe
41.09362468932915	21.05042851027597	45.45403601427674	h
41.72366710528024	17.77971997471785	45.48424633369905	h
43.61525119200733	22.29377676462548	41.79900211632163	h
39.95064371401809	32.37622175347716	34.77255299893115	s
33.05541506953019	33.02834167401368	35.00146030321076	s
47.11499536927711	29.07184794608455	52.74981419527027	o
39.22925283714547	25.16108510888077	36.69843830445544	h
31.89850338505922	39.64509947109008	43.16879773689604	h
37.86224998259367	22.60234938919950	34.97481871636366	h
34.52781381355003	37.53471641359764	43.27849454242640	h
32.47305373188985	37.67924920624719	43.47692895772752	c
30.84997144433573	35.62995323493345	41.18508359563729	s
31.95789967638737	37.11016349135752	45.40776540875370	h
34.37469966921189	18.71753184153734	48.52338693552948	h
36.98201443399613	23.77019948110112	54.22207815796739	h
26.37175151093963	20.96638143552673	46.67854953511313	h

Table 49: Coordinates of isolated Lys358 in bohr.

32.64410217825220	24.82467681308441	47.09531202209317	h
34.56026090686332	25.57774992144361	49.46839747329154	h
35.74232103940317	25.01435269218694	46.61275545730237	h
32.35510269634612	29.36494558506789	47.94307744591937	h
33.97473026629438	28.60423255399947	46.90020751740203	c
34.24771020447012	25.82968202108253	47.56111972754826	n
33.66438177293679	28.75859133357934	44.86160970539976	h
35.71500980104006	29.57716419739289	47.44844272741224	h