

This copy of the ESI replaces the previous version published on 18.06.2021 to update the data availability statement.

## SUPPLEMENTARY INFORMATION

### QM calculations predict the energetics and infrared spectra of transient glutamine isomers in LOV photoreceptors

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### DATA AVAILABILITY STATEMENT.

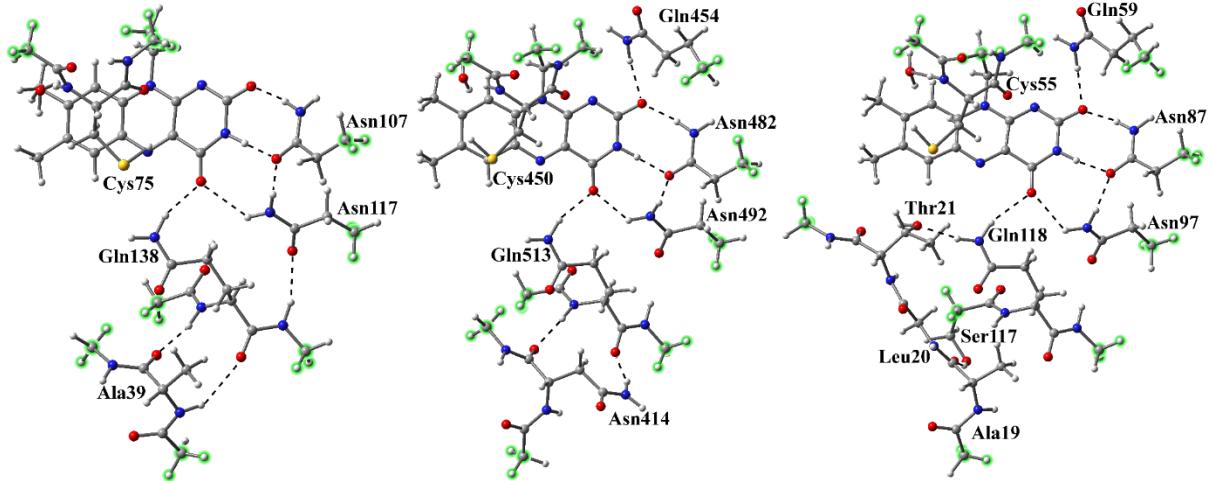
Data for this paper, including time-resolved infrared spectra (Fig. 4) are available at Zenodo at <https://doi.org/10.5281/zenodo.7556678>.

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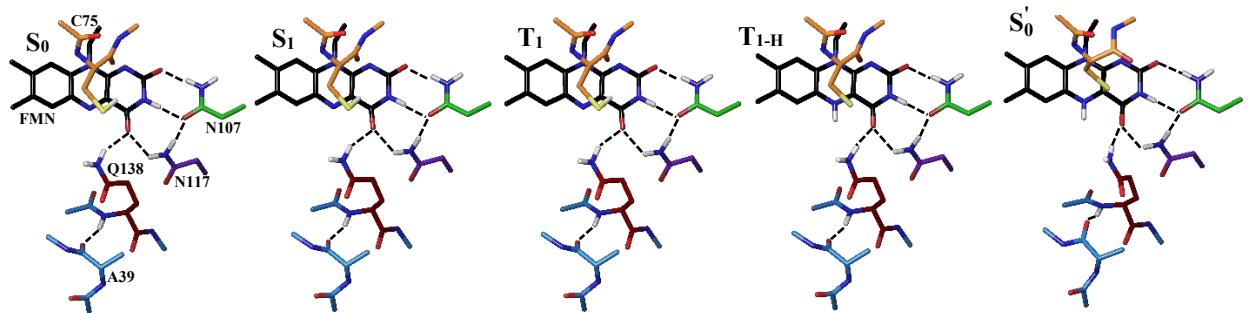
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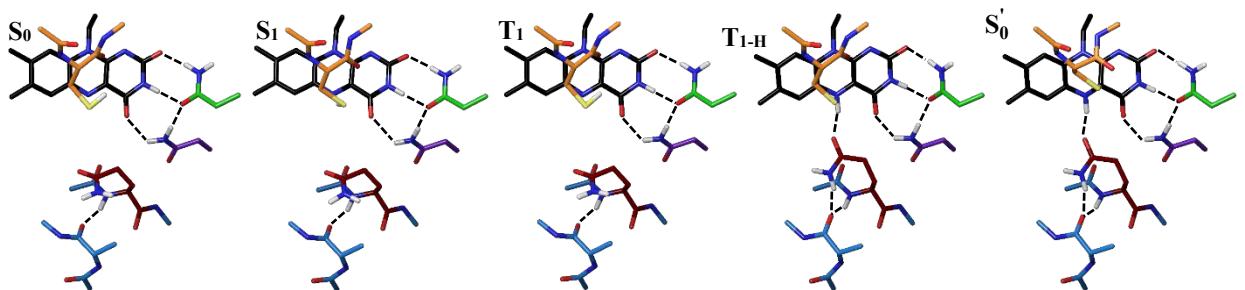
## 1. Electronic and Geometry Data



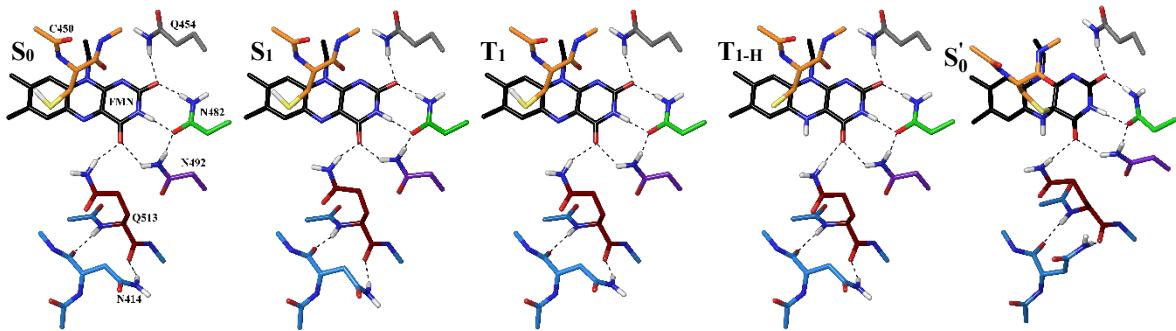
**Figure S1** Optimised structures of the ground state **Qa** models of EL222 (left), AsLOV2 (middle) and RsLOV (right). Fixed atoms to the X-ray positions are highlighted in green and the hydrogen bonding network is displayed with dashed lines.



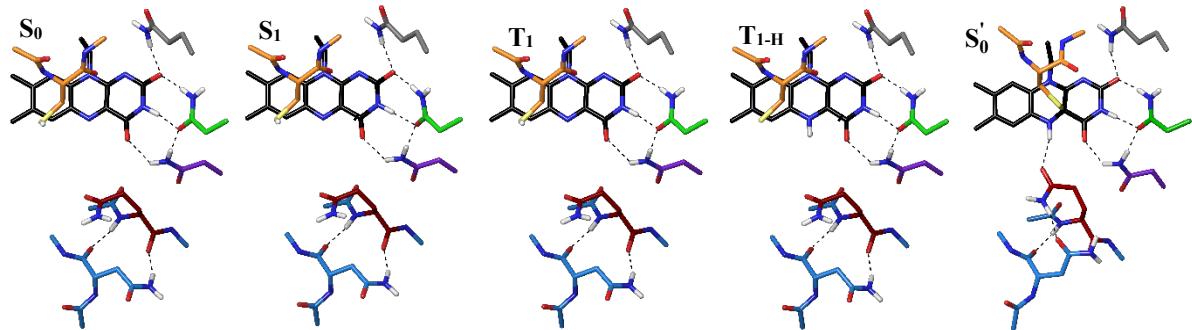
**Figure S2** Optimised **Qa** structures of the EL222 cluster along the reaction coordinate. The hydrogen bonding network is shown with black dashed lines.



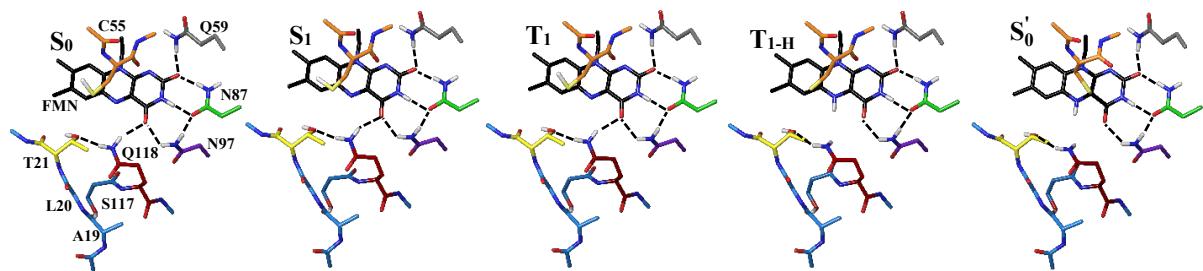
**Figure S3** Optimised **Qc** structures of the EL222 cluster along the reaction coordinate. The hydrogen bonding network is shown with black dashed lines.



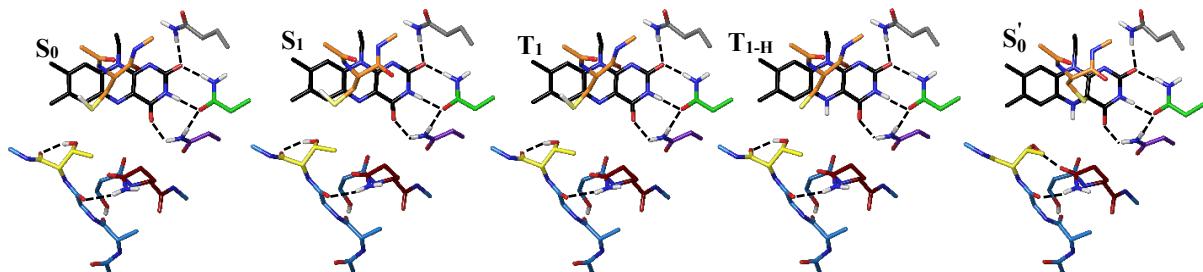
**Figure S4** Optimised **Qa** structures of AsLOV2 along the reaction coordinate. The hydrogen bonding network is shown with black dashed lines.



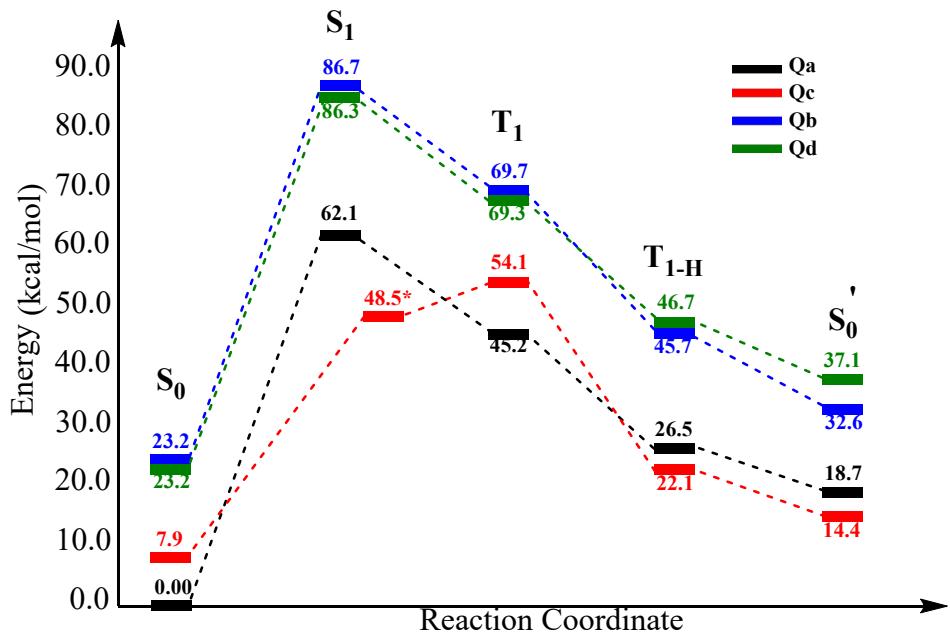
**Figure S5** Optimised **Qc** structures of AsLOV2 along the reaction coordinate. The hydrogen bonding network is shown with black dashed lines.



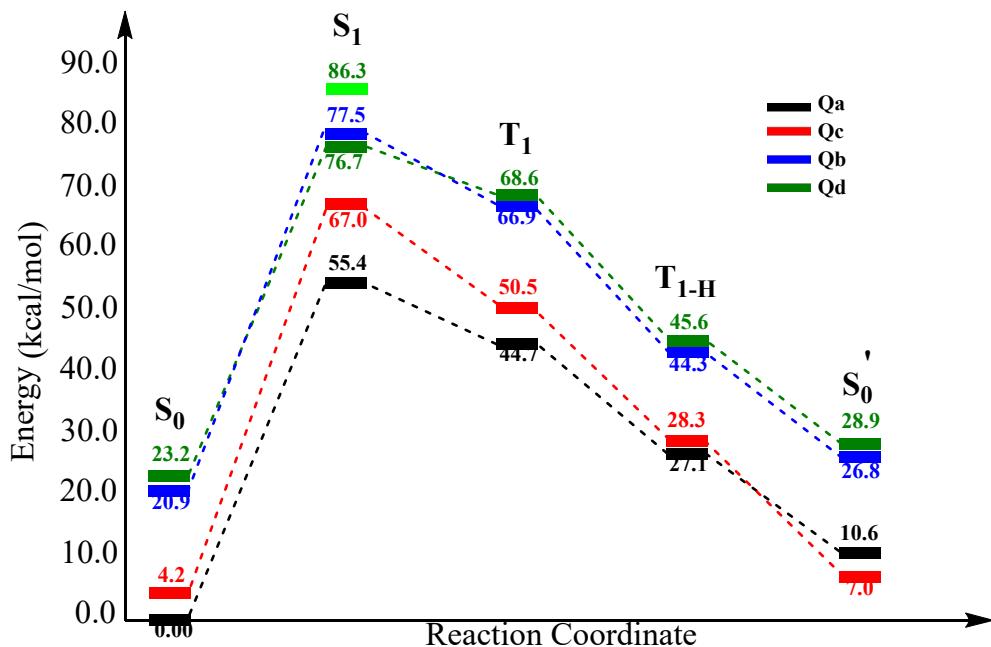
**Figure S6** Optimised **Qa** structures of RsLOV along the reaction coordinate. The hydrogen bonding network is shown with black dashed lines.



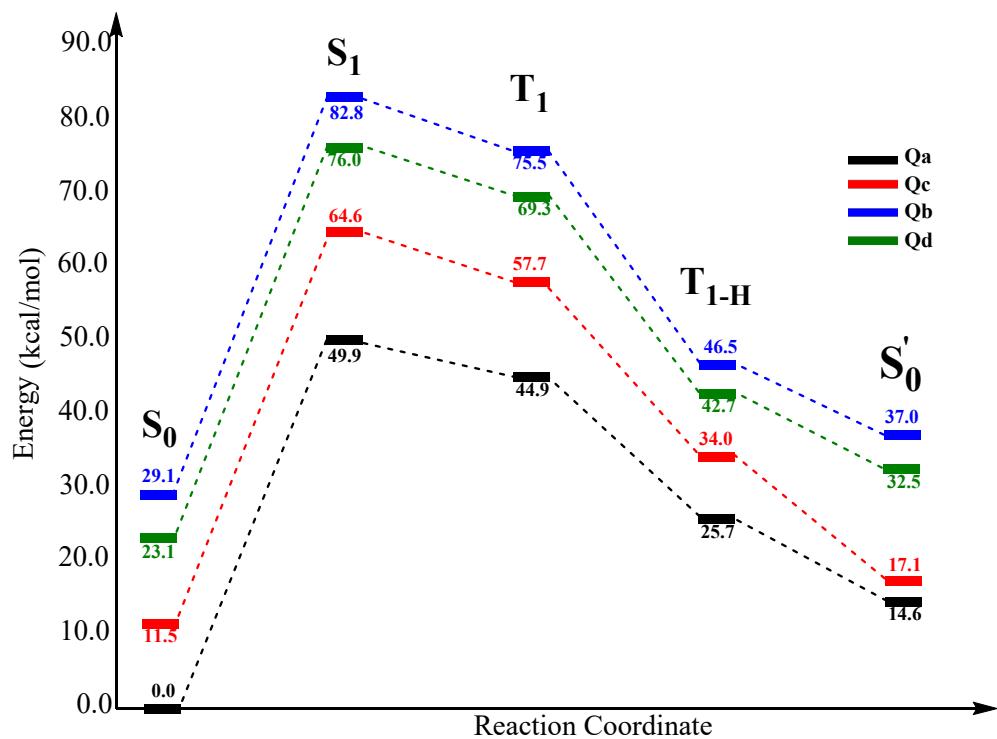
**Figure S7** Optimised **Qc** structures of RsLOV along the reaction coordinate. The hydrogen bonding network is shown with black dashed lines.



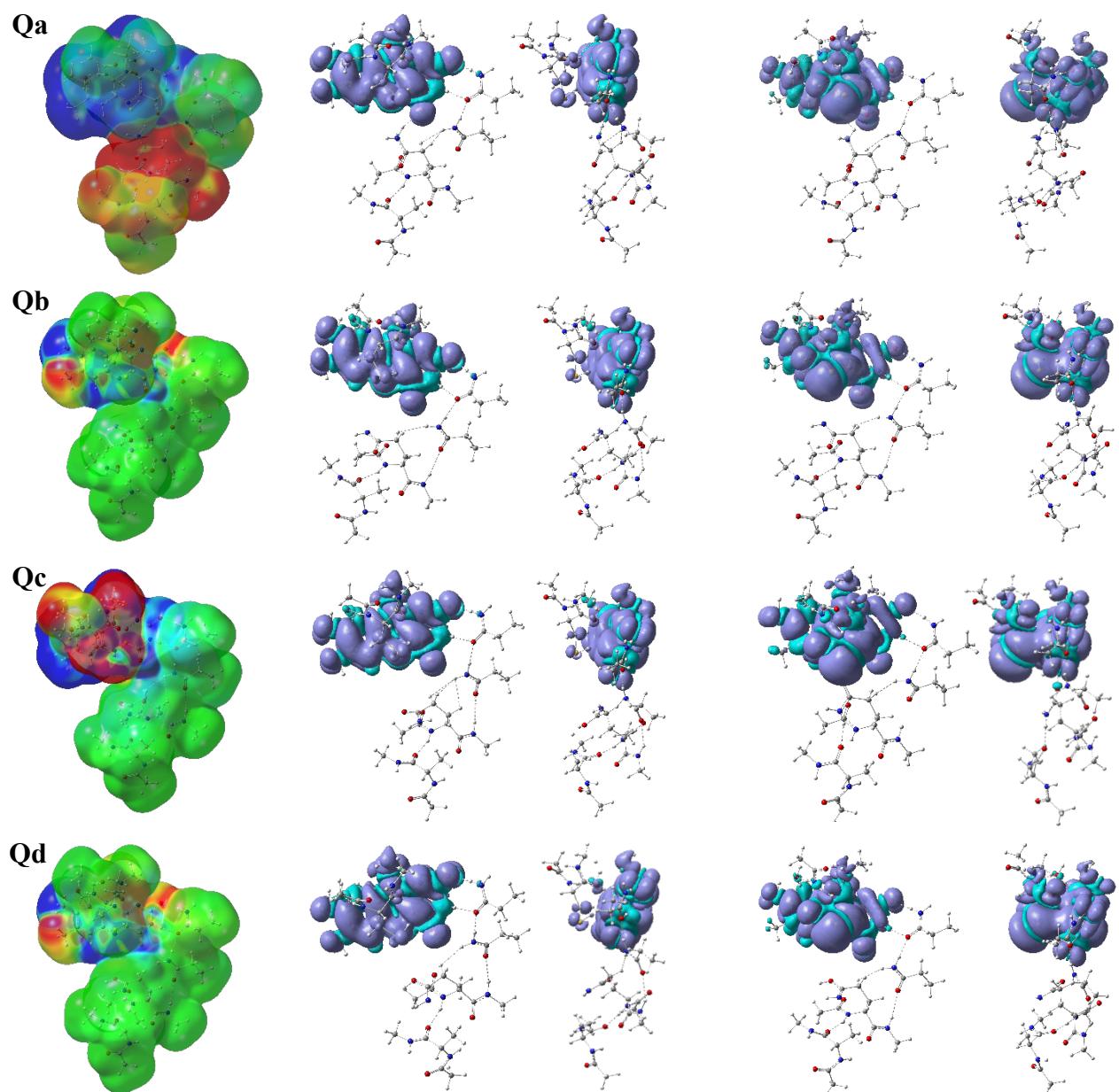
**Figure S8** Relative energies along the reaction path of the EL222 cluster. The imidic Q138 isomers **Qb** and **Qd** are displayed with blue and green, and the amidic **Qa** and **Qc** in black and red respectively. \*: The **Qc**  $S_1$  structure is placed further along the reaction coordinate relative to the rest of the  $S_1$  and  $T_1$  structures (See discussion in Section 3.1 of the main text).



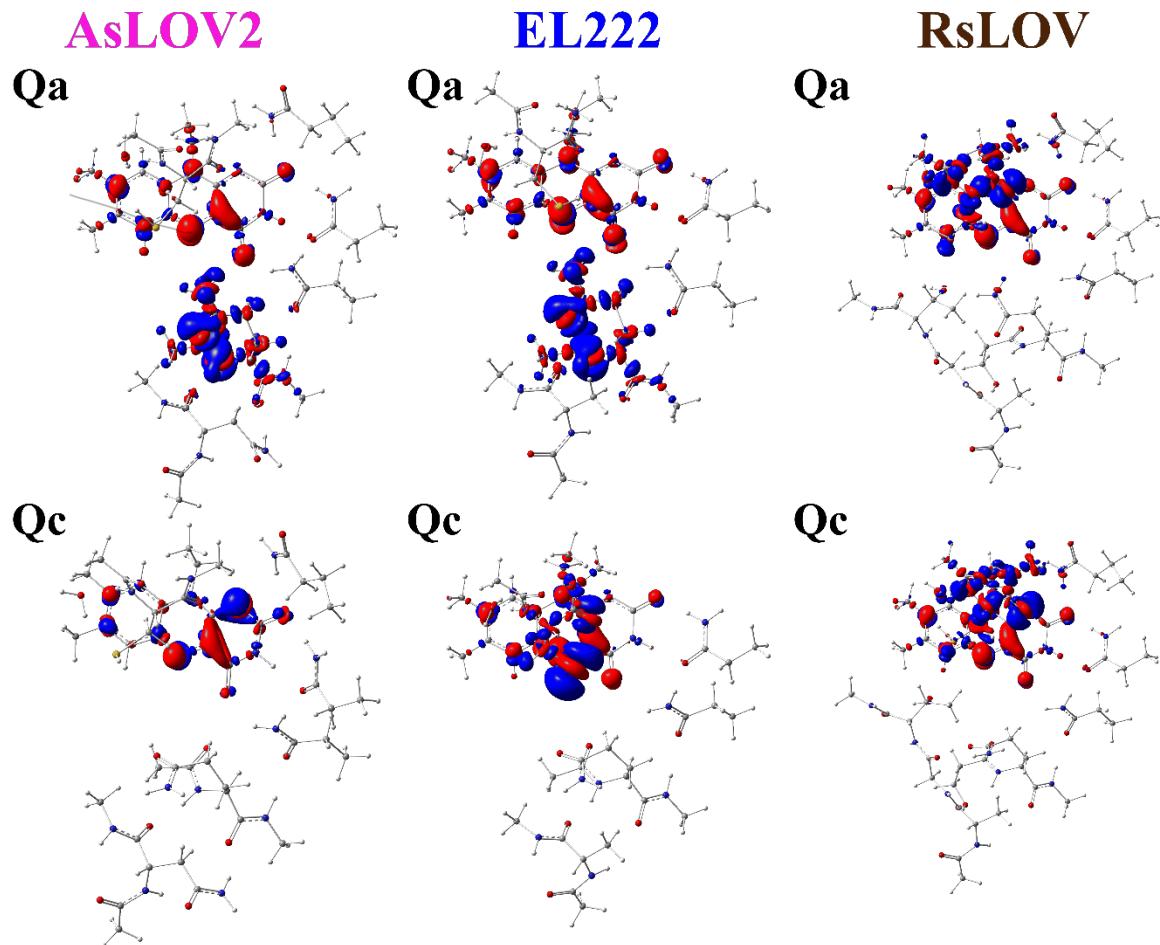
**Figure S9** Relative energies along the reaction path of the AsLOV2 cluster. The imidic Q513 isomers **Qb** and **Qd** are displayed with blue and green, and the amidic **Qa** and **Qc** in black and red respectively. The relative energy of a second  $\pi\pi^*$  degenerate **Qd** excitation is shown in light green.



**Figure S10** Relative energies along the reaction path of the RsLOV cluster. The imidic Q118 isomers **Qb** and **Qd** are displayed with blue and green, and the amidic **Qa** and **Qc** in black and red respectively.



**Figure S11** Left: Electron density difference plots of the  $S_1$  state of the EL222 clusters **Qa-Qd** mapped on the total density. Blue areas indicate positive values *i.e.* where excited state density is larger than the ground state density, and red indicates larger ground state density. Thus, during excitation, electron density moves from the red to the blue area. Middle: Front and side views of spinA-spinB density of the  $T_1$  state of the EL222 cluster models **Qa-Qd**. Right: Front and side views of spinA-spinB density of  $T_1$ -H of the EL222 cluster models **Qa-Qd**.



**Figure S12** Differential electron density plots of the S<sub>1</sub> state of the **Qa** and **Qc** models of EL222, AsLOV2 and RsLOV.

**Table S1** Key distances (in Å) and Q138 sidechain dihedral angle of the EL222 cluster along the reaction coordinate.

	N107 O···HN <sub>3</sub>	N107 NH···O <sub>2</sub>	C75 S···C <sub>4a</sub>	C75 SH···N <sub>5</sub>	N117 NH···O <sub>4'</sub>	Q138 NH···O <sub>4'</sub>	Q138 CCCN	FMN C <sub>2</sub> =O <sub>2</sub>	FMN C <sub>4</sub> =O <sub>4'</sub>
<b>S<sub>0</sub></b>	<b>Qa</b>	1.818	1.894	3.865	2.953	2.126	2.524	-167.5	1.233
	<b>Qb</b>	1.836	1.919	5.270	5.675	2.443	5.257	-131.3	1.235
	<b>Qc</b>	1.815	1.935	5.277	5.480	2.463	5.280	64.6	1.235
	<b>Qd</b>	1.897	1.830	3.924	2.916	2.446	5.977	53.2	1.234
<b>S<sub>I</sub></b>	<b>Qa</b>	1.838	1.910	3.802	2.862	2.449	2.008	-167.9	1.237
	<b>Qb</b>	1.836	1.916	3.860	2.853	2.407	5.454	-132.8	1.238
	<b>Qc</b>	1.891	1.863	3.453	1.674	2.956	5.447	59.5	1.246
	<b>Qd</b>	1.846	1.915	3.843	2.867	2.408	5.945	53.4	1.231
<b>T<sub>I</sub></b>	<b>Qa</b>	1.823	1.920	3.819	2.976	2.501	2.114	-166.8	1.236
	<b>Qb</b>	1.819	1.924	3.917	2.867	2.435	5.458	-132.8	1.237
	<b>Qc</b>	1.821	1.921	3.894	2.897	2.452	5.332	58.9	1.237
	<b>Qd</b>	1.829	1.919	3.887	2.914	2.442	5.939	53.5	1.230
<b>T<sub>I-II</sub></b>	<b>Qa</b>	1.830	1.856	3.804	1.018	2.575	1.993	-178.4	1.239
	<b>Qb</b>	1.824	1.851	3.658	1.022	2.397	4.836	-141.4	1.241
	<b>Qc</b>	1.803	1.882	3.760	1.038	2.158	5.551	16.4	1.243
	<b>Qd</b>	1.835	1.857	3.658	1.019	2.429	5.856	47.9	1.240
	<b>TS</b>	1.845	1.850	3.625	1.019	2.555	4.206	94.0	1.240
<b>S<sub>II</sub></b>	<b>Qa</b>	1.856	1.851	1.943	1.017	2.618	2.048	-165.3	1.228
	<b>Qb</b>	1.797	1.836	1.948	1.020	2.541	4.398	-127.9	1.230
	<b>Qc</b>	1.753	1.841	1.968	1.030	2.508	5.319	23.3	1.232
	<b>Qd</b>	1.856	1.841	1.945	1.018	2.663	5.602	48.2	1.229
	<b>TS</b>	1.792	1.852	1.943	1.018	2.596	2.438	113.6	1.229

**Table S2** Key distances (in Å) and Q513 sidechain dihedral angle of the AsLOV2 cluster along the reaction coordinate.

	N482 O···HN <sub>3</sub>	N482 NH···O <sub>2</sub>	Q454 NH···O <sub>2</sub>	C450 S···C <sub>4a</sub>	C450 SH···N <sub>5</sub>	N492 NH···O <sub>4'</sub>	Q513 NH···O <sub>4'</sub>	Q513 CCCN	FMN C <sub>2</sub> =O <sub>2'</sub>	FMN C <sub>4</sub> =O <sub>4'</sub>	
S <sub>0</sub>	<b>Qa</b>	1.776	1.900	2.033	5.093	5.304	2.469	2.075	-171.5	1.242	1.229
	<b>Qb</b>	1.836	1.919	2.040	5.270	5.675	2.443	5.257	-131.3	1.242	1.222
	<b>Qc</b>	1.815	1.936	1.992	5.277	5.480	2.463	5.280	64.6	1.245	1.224
	<b>Qd</b>	1.811	1.928	1.997	5.235	4.971	2.473	5.953	50.9	1.245	1.223
S <sub>1</sub>	<b>Qa</b>	1.893	1.819	1.926	5.099	5.313	2.397	1.858	176.8	1.261	1.252
	<b>Qb</b>	2.023	1.846	2.006	5.457	5.870	1.743	5.302	-135.2	1.261	1.254
	<b>Qc</b>	1.859	1.938	2.016	5.186	5.380	2.390	5.248	64.1	1.245	1.232
	<b>Qd</b>	1.875	1.904	2.019	5.065	4.739	2.448	5.857	51.6	1.246	1.231
T <sub>1</sub>	<b>Qd2</b>	1.956	1.866	1.905	5.290	5.790	2.395	5.918	51.7	1.261	1.237
	<b>Qa</b>	1.771	1.927	2.040	5.043	5.290	2.450	2.067	-172.7	1.243	1.236
	<b>Qb</b>	1.829	1.938	2.039	5.177	5.565	2.442	5.243	-130.7	1.243	1.229
	<b>Qc</b>	1.810	1.952	2.016	5.204	5.414	2.456	5.216	64.2	1.246	1.230
T <sub>1-2</sub>	<b>Qd</b>	1.798	1.938	2.026	5.144	4.956	2.499	5.893	51.3	1.244	1.229
	<b>Qa</b>	1.793	1.866	2.006	5.034	1.018	2.581	2.010	-178.7	1.248	1.245
	<b>Qb</b>	1.846	1.896	2.022	5.244	1.021	2.384	5.023	-138.3	1.248	1.238
	<b>Qc</b>	1.824	1.912	1.967	5.107	1.019	2.437	5.344	63.8	1.250	1.239
T <sub>2</sub>	<b>Qd</b>	1.858	1.911	2.014	5.141	1.020	2.349	5.929	43.0	1.248	1.239
	<b>TS</b>	1.788	1.876	1.978	5.067	1.019	2.624	3.251	99.4	1.250	1.240
	<b>Qa</b>	1.762	1.868	2.020	1.953	1.021	2.373	2.207	148.0	1.237	1.226
	<b>Qb</b>	1.765	1.872	2.007	1.966	1.029	2.271	4.338	-164.1	1.238	1.221
S <sub>2</sub>	<b>Qc</b>	1.755	1.877	2.001	1.966	1.026	2.284	5.321	23.1	1.239	1.221
	<b>Qd</b>	1.753	1.874	2.012	1.950	1.021	2.314	5.427	5.7	1.238	1.221
	<b>TS</b>	1.784	1.848	2.003	1.949	1.017	2.358	5.311	55.4	1.238	1.221

**Table S3** Key distances (in Å) and Q118 sidechain dihedral angle of the RsLOV cluster along the reaction coordinate.

	N87 O···HN <sub>3</sub>	N87 NH···O <sub>2</sub>	Q59 NH···O <sub>2</sub>	C55 S···C <sub>4a</sub>	C55 SH···N <sub>5</sub>	N97 NH···O <sub>4'</sub>	Q118 NH···O <sub>4'</sub>	Q118 CCCN	FMN C <sub>2</sub> =O <sub>2</sub>	FMN C <sub>4</sub> =O <sub>4'</sub>
S <sub>0</sub>	Qa	1.822	1.823	1.923	5.093	5.317	2.363	2.340	-156.8	1.242
	Qb	1.796	1.831	1.904	5.106	5.340	2.429	5.379	-119.9	1.245
	Qc	1.826	1.822	1.907	5.080	5.325	2.418	5.173	73.3	1.244
	Qd	1.781	1.837	1.907	5.090	5.295	2.376	5.761	19.0	1.244
S <sub>i</sub>	Qa	1.930	1.781	1.822	5.224	5.086	2.214	2.110	-163.8	1.260
	Qb	1.883	1.757	1.808	4.802	4.484	2.358	5.351	-116.9	1.263
	Qc	1.925	1.749	1.812	4.780	4.461	2.346	4.963	77.5	1.263
	Qd	1.871	1.760	1.812	4.796	4.368	2.324	5.593	24.8	1.263
T <sub>i</sub>	Qa	1.818	1.843	1.936	5.040	5.304	2.325	2.330	-157.8	1.244
	Qb	1.791	1.850	1.919	5.049	5.313	2.409	5.373	-118.3	1.246
	Qc	1.821	1.840	1.923	5.019	5.300	2.401	5.101	75.64	1.246
	Qd	1.784	1.855	1.922	5.035	5.253	2.348	5.703	19.6	1.246
T <sub>i-H</sub>	Qa	1.823	1.793	1.892	5.096	1.022	2.346	3.653	-136.7	1.249
	Qb	1.756	1.813	1.874	5.229	1.047	2.141	4.195	-157.6	1.252
	Qc	1.848	1.792	1.892	5.083	1.020	2.381	5.193	70.4	1.249
	Qd	1.775	1.808	1.888	5.126	1.026	2.245	5.613	11.0	1.250
S <sub>0</sub> '	Qa	1.851	1.785	1.936	1.938	1.020	2.381	3.572	-133.8	1.237
	Qb	1.786	1.781	1.928	1.953	1.025	2.313	4.440	-138.7	1.239
	Qc	1.824	1.790	1.934	1.943	1.018	2.355	5.177	59.8	1.238
	Qd	1.808	1.789	1.932	1.941	1.022	2.320	5.540	19.8	1.238

**Table S4** Mulliken charges of the isoalloxazine moiety of the EL222, AsLOV2 and RsLOV cluster models **Qa-Qd** along the reaction coordinate.

	S <sub>0</sub>	S <sub>1</sub>	T <sub>1</sub>	T <sub>1-H</sub>	S <sub>0'</sub>
EL222	Qa	0.031	-0.050	0.032	0.037
	Qb	-0.019	-0.017	-0.021	-0.008
	Qc	-0.016	-0.700	-0.019	-0.081
	Qd	-0.018	-0.017	-0.021	0.000
AsLOV2	Qa	0.081	0.142	0.055	0.080
	Qb	0.049	0.133	0.029	0.072
	Qc	0.002	0.006	-0.012	0.088
	Qd	0.020	0.057	0.013	0.081
RsLOV	Qa	-0.014	0.046	-0.042	-0.051
	Qb	-0.044	0.042	-0.065	-0.076
	Qc	-0.053	0.035	-0.074	-0.039
	Qd	-0.038	0.038	-0.066	-0.049

## 2a. Vibrational Data (Non-Deuterated Spectra)

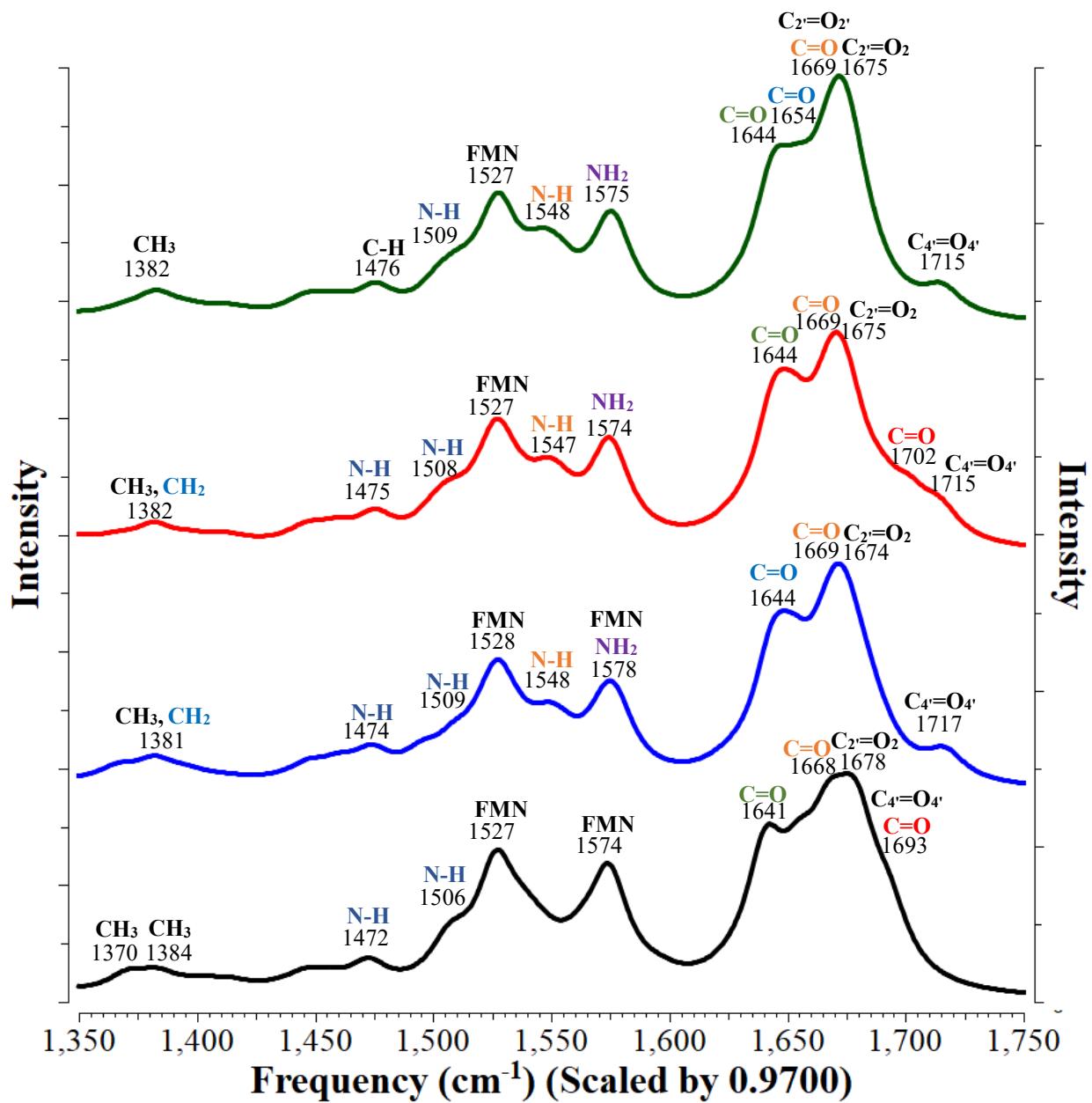
A brief description of the computed spectra not discussed in the main text is given here:

**EL222:** The **Qc** S<sub>1</sub> of EL222 was established as a CT state so it is not discussed in the main text. Due to the flip of the Q138 side chain, the carbonyl stretch is blueshifted to 1698 cm<sup>-1</sup>, while the amide peak, uncoupled to other modes, is found at 1553 cm<sup>-1</sup> (non-deuterated value). When glutamine tautomerises, as in **Qb**, a unique weak-to-medium shoulder appears at 1664 cm<sup>-1</sup> due to the C=N stretch, and another weak peak at 1259 cm<sup>-1</sup> due to the H-rocking of the HOCONH (DOCND) imidic moiety which is downshifted due to the deuteration ([Table S7](#)). Similarly, in **Qd**, the former appears at 1658 cm<sup>-1</sup> with weaker intensity, displaying also sensitivity to the side chain rotation, and the latter at 1242 cm<sup>-1</sup> with matching intensity. A unique feature of the non-deuterated T<sub>1-H</sub> spectra (and the subsequent adduct S<sub>0'</sub>) is the N<sub>5</sub>-H bending mode, which appears throughout the fingerprint region, from 1600 cm<sup>-1</sup> down to 1390 cm<sup>-1</sup> coupled to other modes. This mode downshifts below 1350 cm<sup>-1</sup> in deuterium. Adduct formation (and H-transfer) can be traced by the appearance of a negative peak in the transparent window, due to the disappearance of the S-H(D) mode of cysteine (~2600 cm<sup>-1</sup>). It was shown that, leading to the H-transfer TS, the peak can shift to as low a wavenumber as 1800 cm<sup>-1</sup>. (S<sub>1</sub> **Qc**). These peaks are expected to downshift by 800 cm<sup>-1</sup> in deuterium.

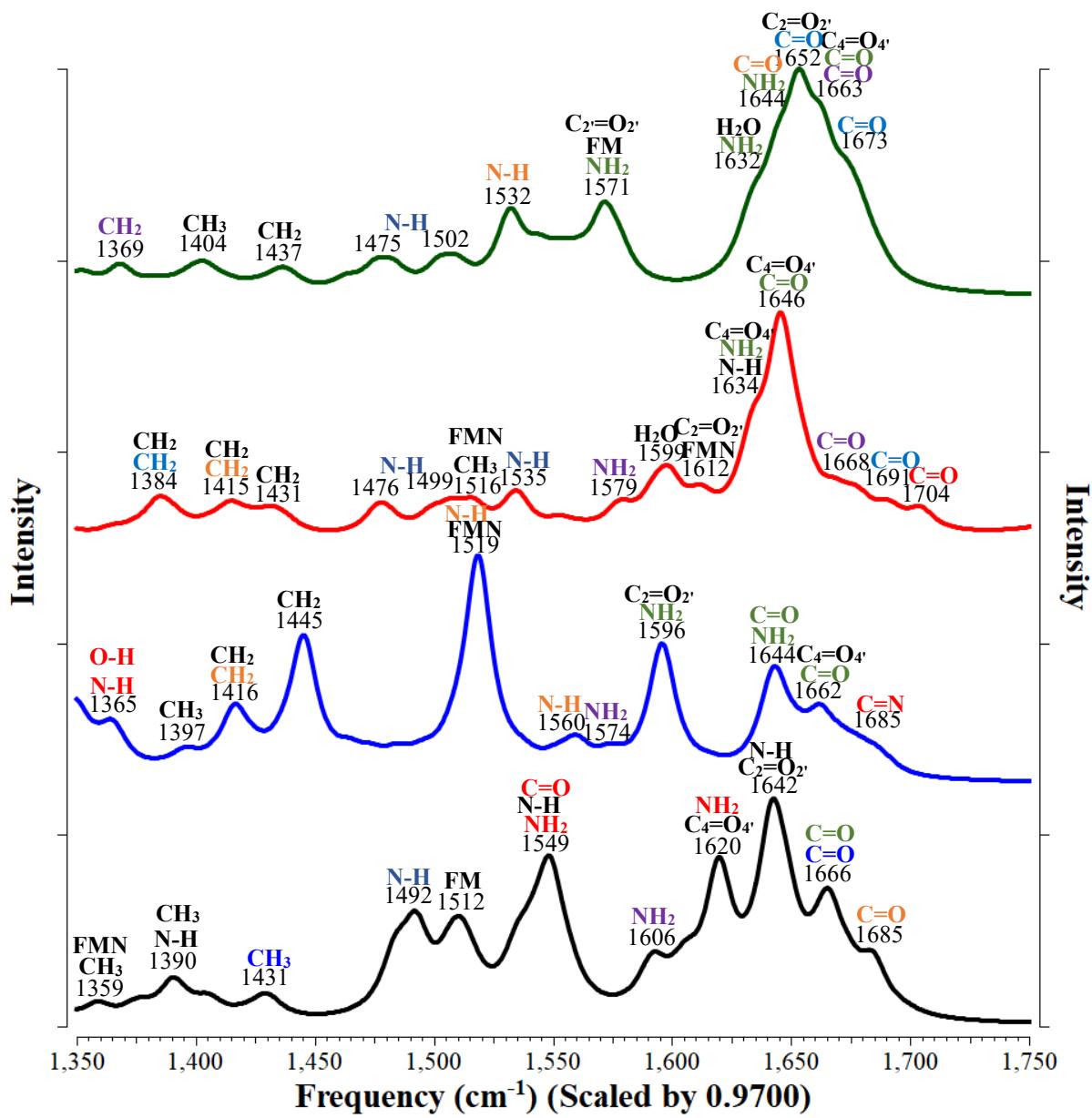
**AsLOV2:** In the AsLOV2 S<sub>1</sub> **Qc** spectrum, the side chain glutamine carbonyl stretch is predicted at 1691 cm<sup>-1</sup> with medium intensity decoupled from the ND<sub>2</sub> mode, which downshifts to 1115 cm<sup>-1</sup> with weak intensity. With regards to the imidic isomers, **Qb** displays a weak C=N stretch at 1666 cm<sup>-1</sup> and **Qd** at 1661 cm<sup>-1</sup> with medium intensity ([Table S7](#)). The HNCOH bending modes span 1360-1380 cm<sup>-1</sup> with weak intensity for all species up to and including the adduct and redshift substantially upon deuteration. In the adduct and T<sub>1-H</sub> spectra, the bending mode of the newly formed N<sub>5</sub>-H is registered in many different vibrations, as in EL222, spanning the whole 1350-1750 cm<sup>-1</sup> region. As mentioned above, upon deuteration, these uncouple from fingerprint vibrations and shift to the red of the studied region.

**RsLOV:** Compared to EL222 and AsLOV2, unique weak-to-medium peaks arise from the hydroxy group of the additional threonine residue at 1650 cm<sup>-1</sup> coupled to the adjacent backbone C=O stretch, and at 1390 cm<sup>-1</sup> of weak relative intensity. These are predicted to downshift below 1350 cm<sup>-1</sup> in D<sub>2</sub>O.

Overall, imidic tautomerisation peaks include C=N stretching and HOCONH bending modes. Both are of weak intensity and are located around 1680 and 1360 cm<sup>-1</sup>, respectively with the latter expected to disappear from the fingerprint region in D<sub>2</sub>O. Thus, possible tautomerisation could be better tracked indirectly by the disappearance of the glutamine carbonyl and amide modes. Amide labelling and double difference spectra are required to reveal imidic vibrations in the experimental spectra, as was shown in BLUF.



**Figure S13** Calculated non-deuterated infrared spectra of the ground state  $S_0$  of the EL222 cluster. The spectra of the amidic Q138 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q138 red, to C75 orange, to N107 green, to N117 violet and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of 8  $\text{cm}^{-1}$ .



**Figure S14** Calculated non-deuterated infrared spectra of the S<sub>1</sub> state of the EL222 cluster. The spectra of amidic Q138 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q138 red, to C75 orange, to N107 green, to N117 violet and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of 8 cm<sup>-1</sup>.

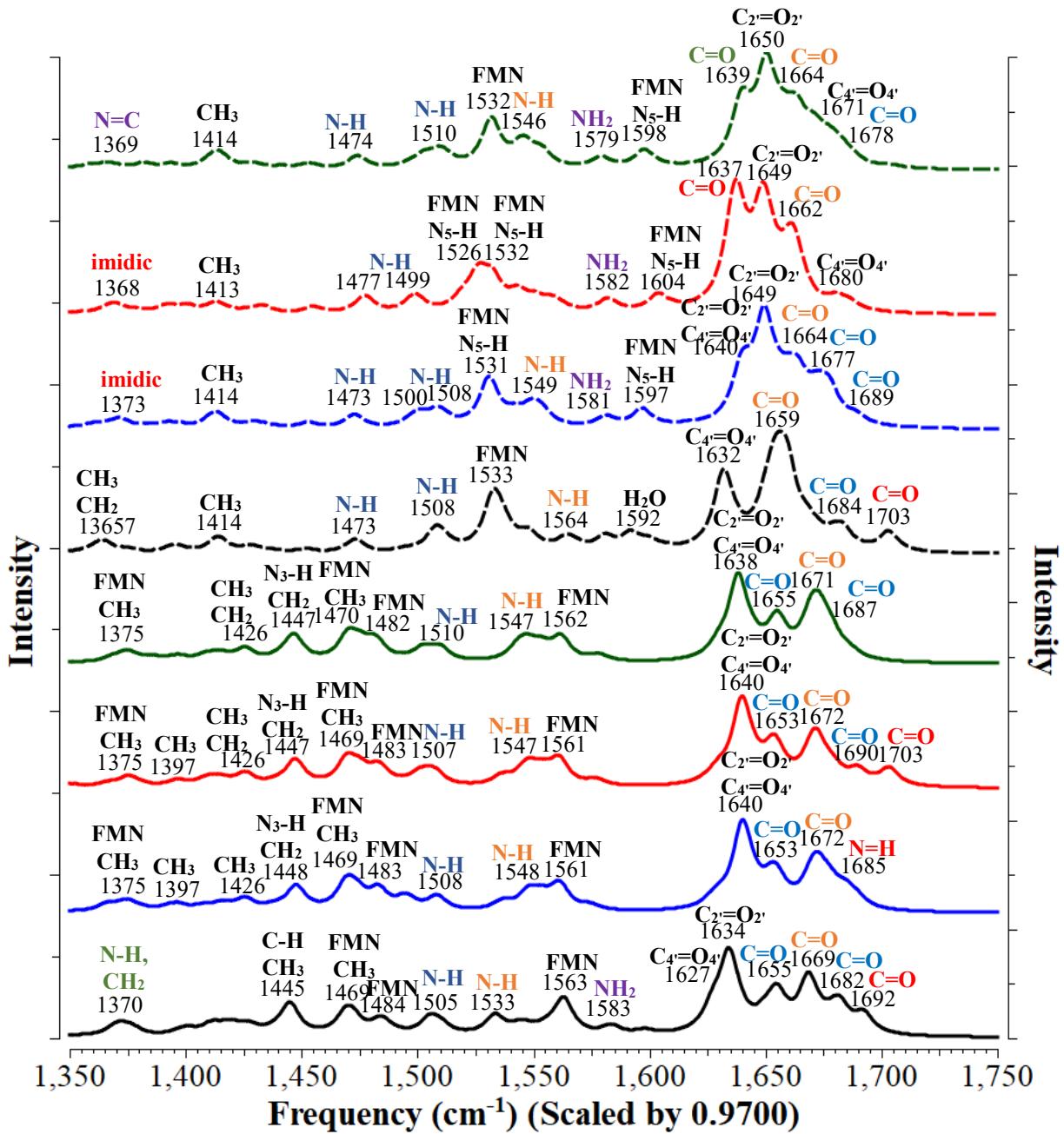
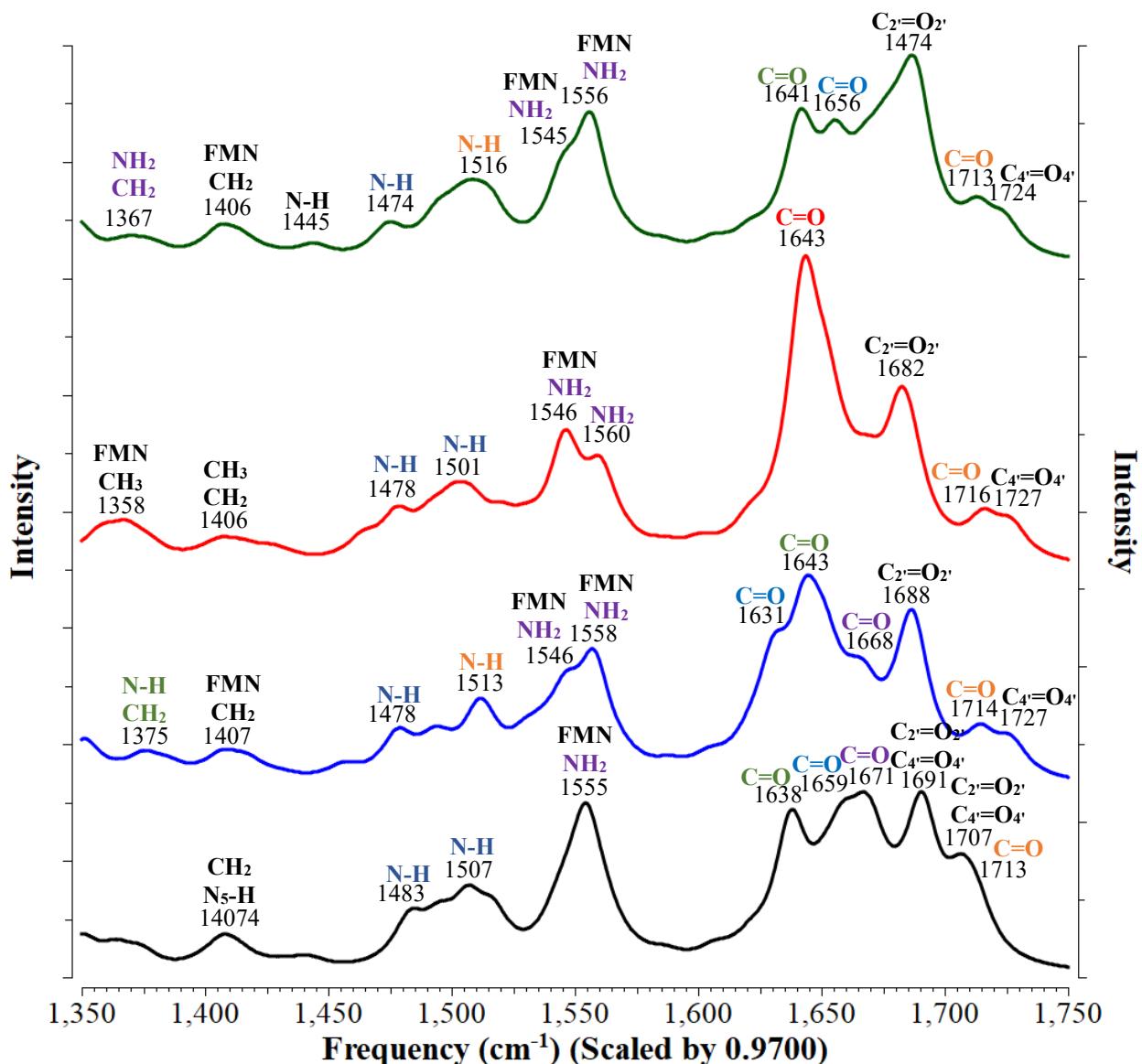
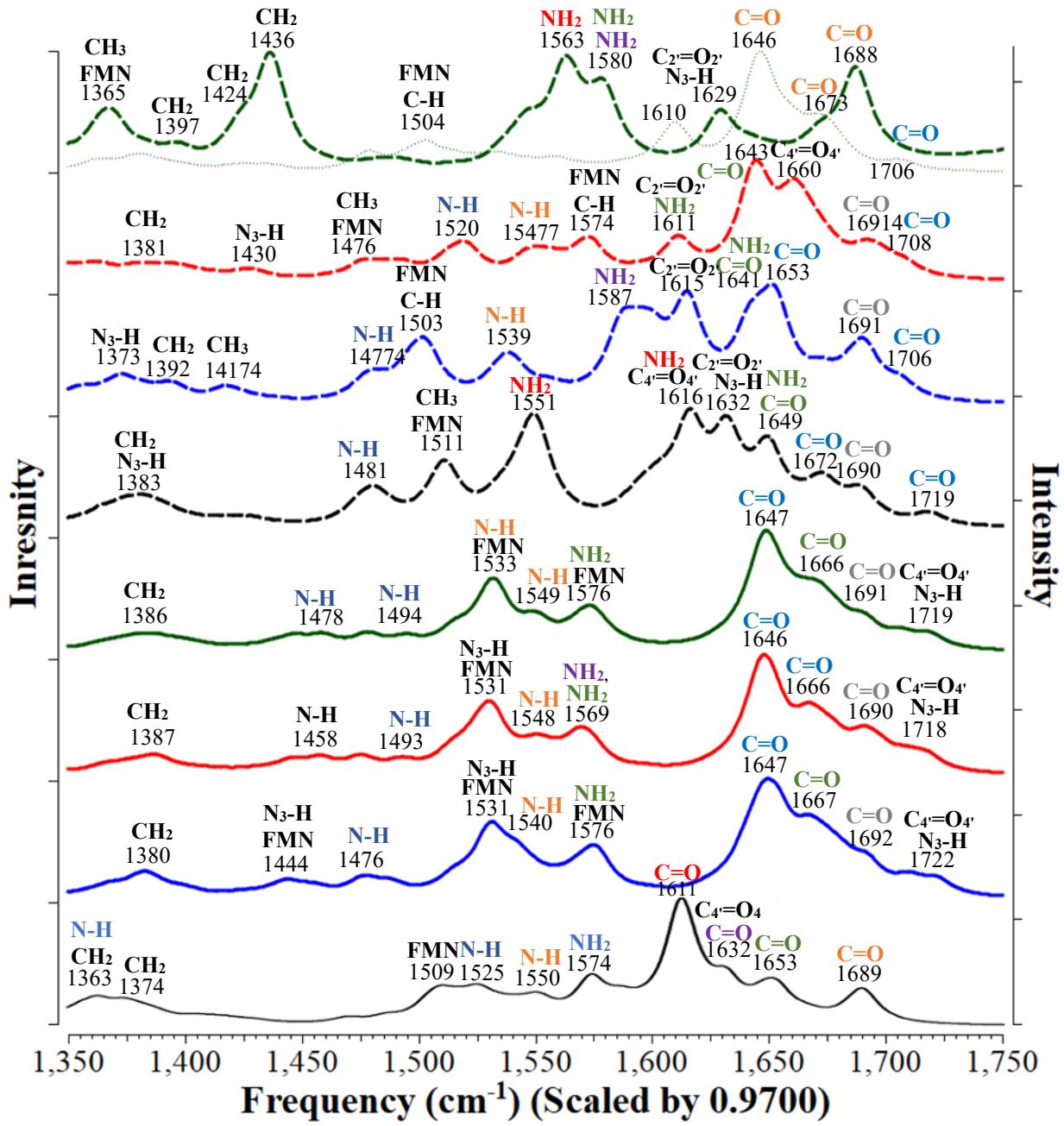


Figure S15 Calculated non-deuterated infrared spectra of the  $T_1$  (solid lines) and  $T_{1\text{-}H}$  states (dashed lines) of the EL222 cluster. The spectra of the amidic Q138 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q138 red, to C75 orange, to N107 green, to N117 violet and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$ .



**Figure S16** Calculated non-deuterated infrared spectra of the adduct state  $S_0'$  of the EL222 cluster. The spectra of amidic Q138 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q138 red, to C75 orange, to N107 green, to N117 violet and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of  $8\text{ cm}^{-1}$ .



**Figure S17** Calculated non-deuterated infrared spectra of the  $S_0$  (solid lines) and  $S_1$  states (dashed lines) of the AsLOV2 cluster. The spectra of the amidic Q513 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. The infrared spectrum of the second  $\pi\pi^*$  excitation of **Qd** is also included with a green dotted line. Vibrations assigned to FMN normal modes are labelled black, to Q513 red, to C450 orange, to N482 green, to N492 violet, to Q454 grey and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$ .

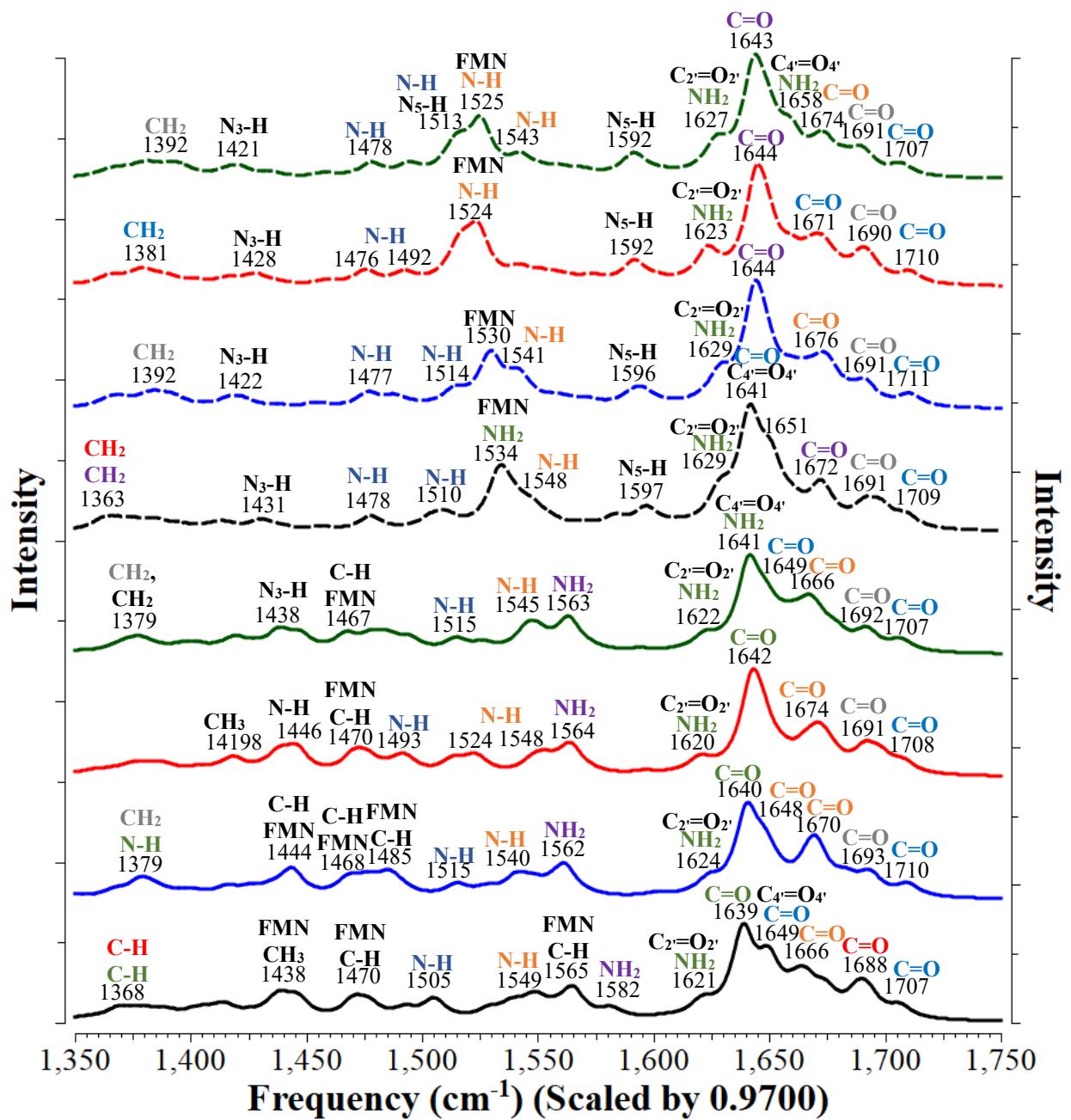
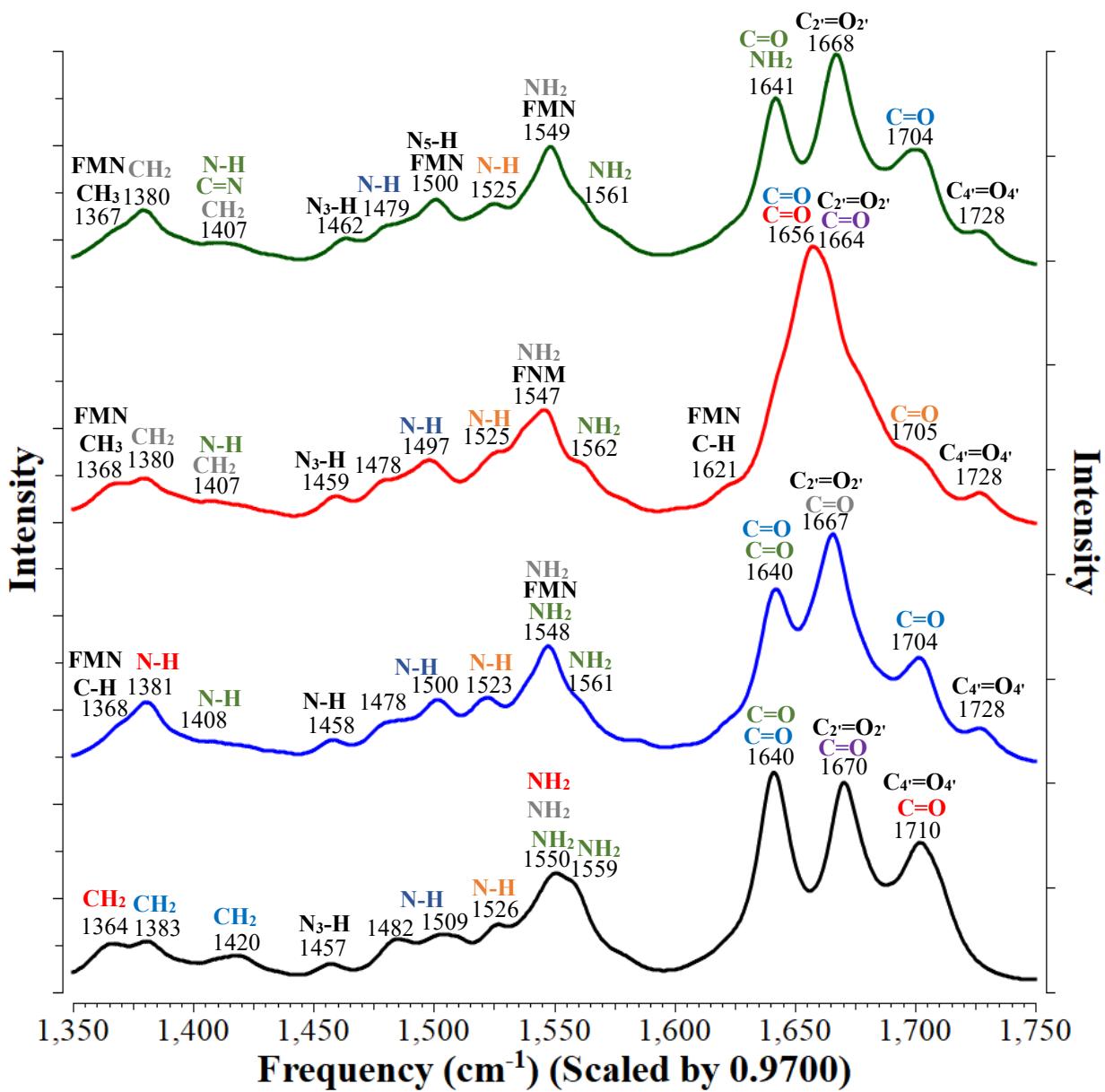
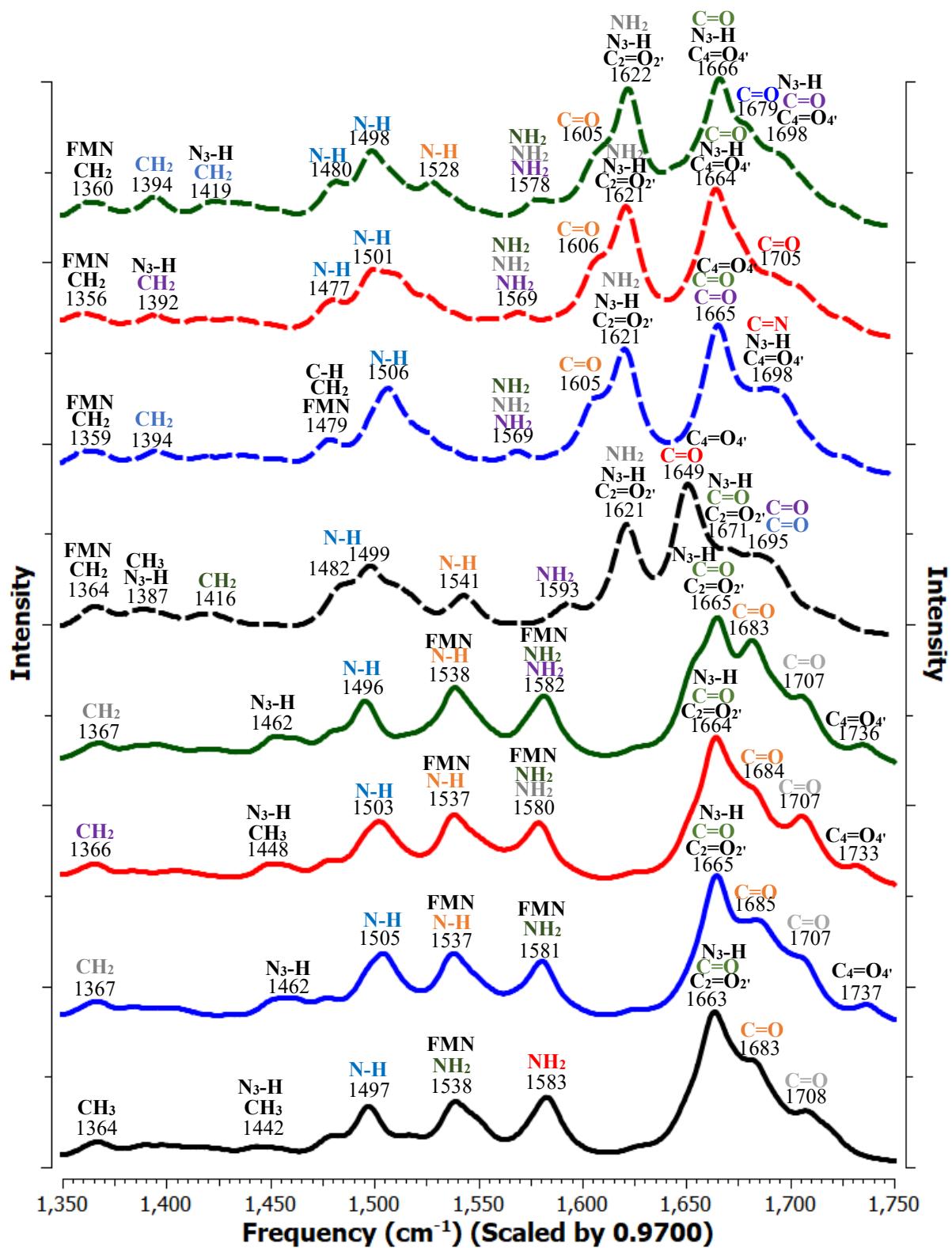


Figure S18 Calculated non-deuterated infrared spectra of the T<sub>1</sub> (solid lines) and T<sub>1-H</sub> states (dashed lines) of the AsLOV2 cluster. The spectra of the amidic Q513 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q513 red, to C450 orange, to N482 green, to N492 violet, to Q454 grey and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of 8  $\text{cm}^{-1}$ .



**Figure S19** Calculated non-deuterated infrared spectra of the adduct state ( $S_0'$ ) of the AsLOV2 cluster. The spectra of the amidic Q513 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q513 red, to C450 orange, to N482 green, to N492 violet, to Q454 grey and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$ .



**Figure S20** Calculated non-deuterated infrared spectra of the S<sub>0</sub> (solid) and S<sub>1</sub> states (dashed) lines of the RsLOV cluster. The spectra of the amidic Q118 models **Qa** and **Qc** are shown with black and red, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q118 red, to C55 orange, to N87 green, to N97 violet, to Q59 grey, to T21 yellow, and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of 8 cm<sup>-1</sup>.

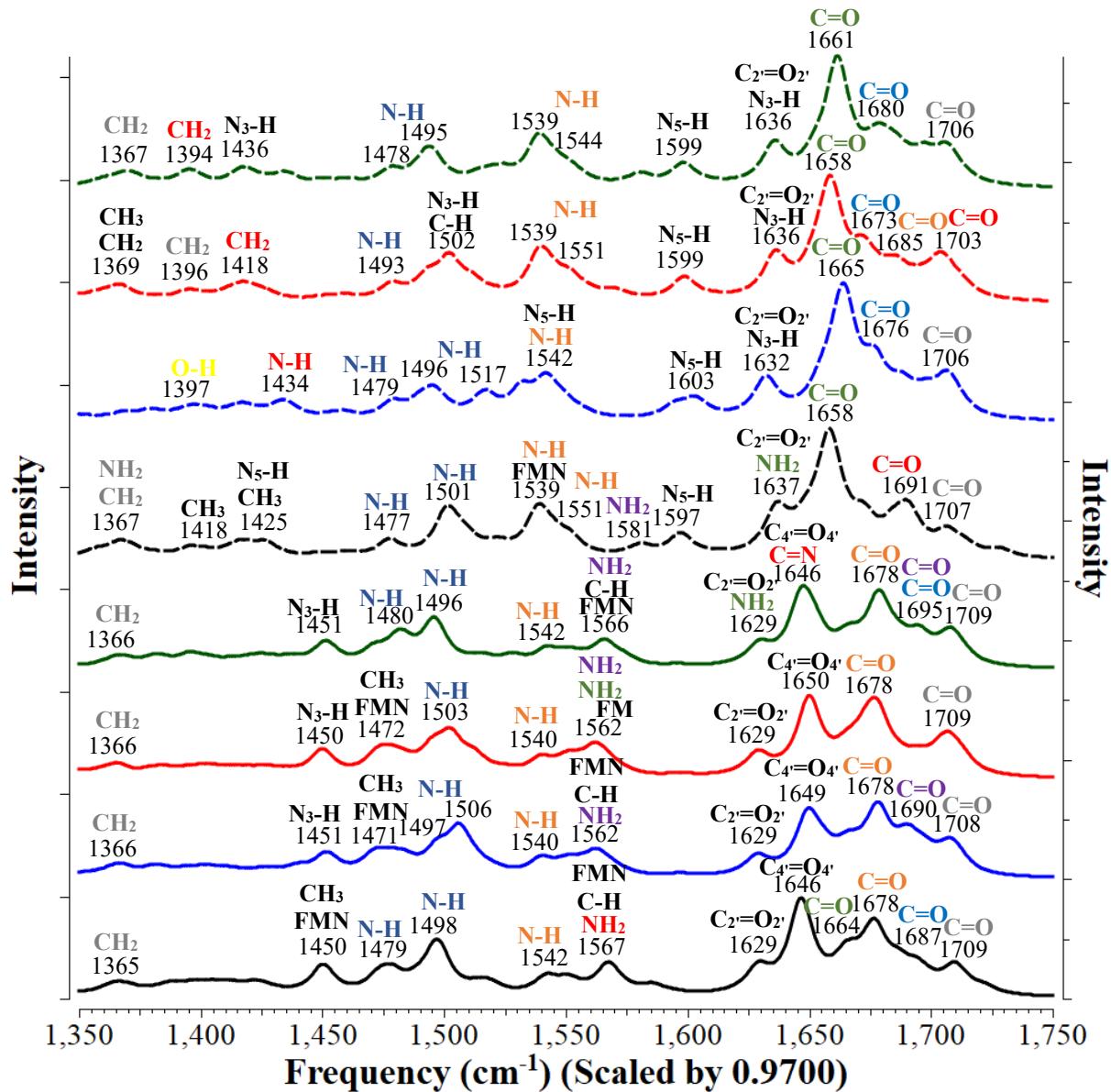


Figure S21 Calculated non-deuterated infrared spectra of the T<sub>1</sub> (solid lines) and T<sub>1</sub>-H states (dashed lines) of the RsLOV cluster. The spectra of the amidic Q118 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q118 red, to C55 orange, to N87 green, to N97 violet, to Q59 grey, to T21 yellow, and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of 8 cm<sup>-1</sup>.

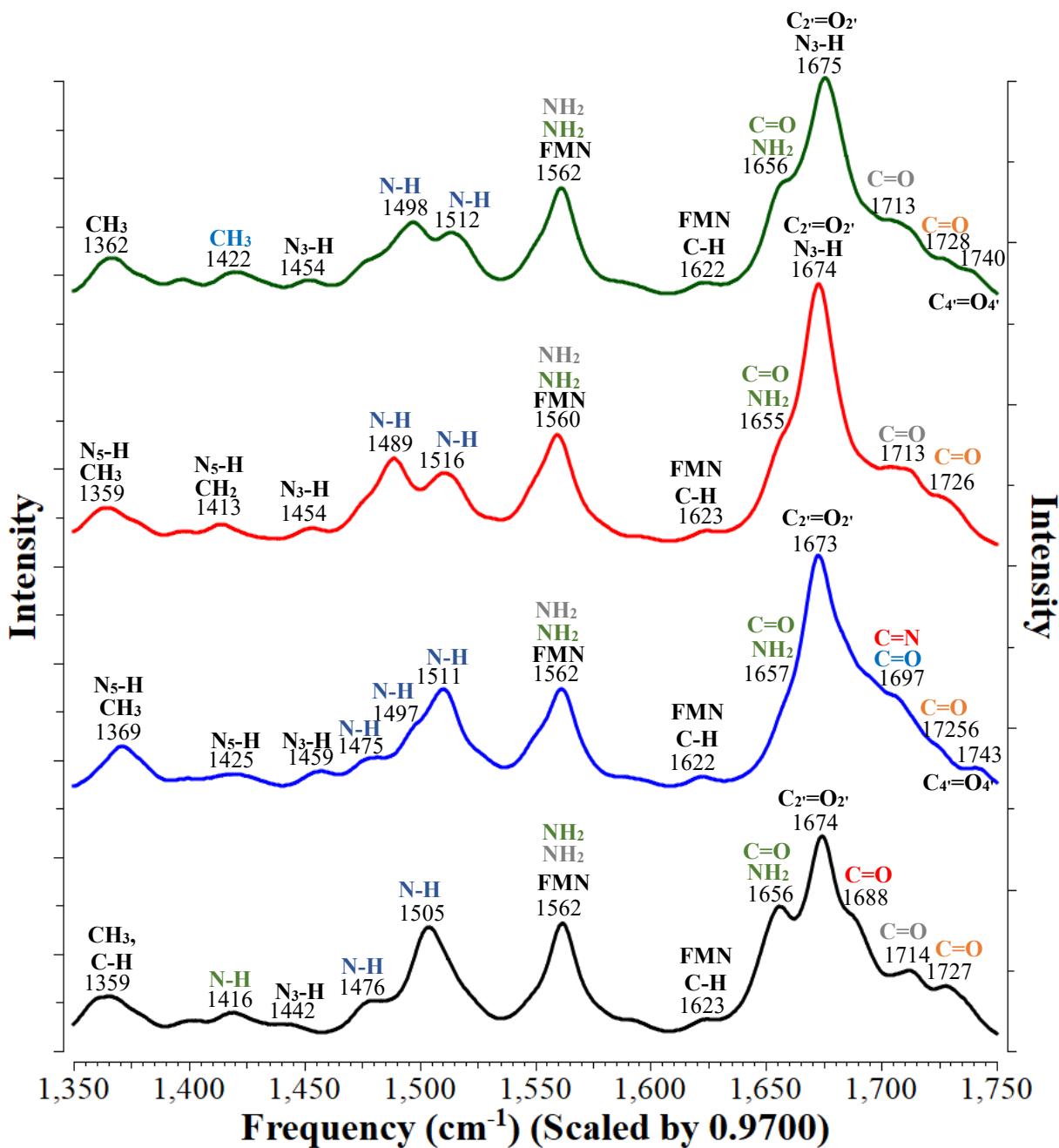


Figure S22 Calculated non-deuterated infrared spectra of the adduct state ( $S_0'$ ) of the RsLOV cluster. The spectra of the amidic Q118 models **Qa** and **Qc** are shown with black and red lines, and of the imidic isomers **Qb** and **Qd** with blue and green, respectively. Vibrations assigned to FMN normal modes are labelled black, to Q118 red, to C55 orange, to N87 green, to N97 violet, to Q59 grey, to T21 yellow, and to other backbone modes, blue. All spectra were drawn with a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$ .

**Table S5** Assignment Table for major vibrations of the EL222 cluster. Values for the non-deuterated spectra in  $\text{cm}^{-1}$ .

		C=O	C=O	C=N	CHNH	C=O	C=O	C <sub>4</sub> =O <sub>4</sub>	C <sub>2</sub> =O <sub>2</sub>	C=O	NH <sub>2</sub>	NH <sub>2</sub>	NH <sub>2</sub>	N <sub>5</sub> -H	N <sub>3</sub> -H	N-H	N-H	CH <sub>3</sub>	CH <sub>2</sub>	C-H	FMN	H <sub>2</sub> O									
S <sub>0</sub> <b>Qa</b>	1641	1693	-	-	1683	1655	1666	1693	1678	1668	1641	1584	1574	-	1678	1457	1506	1472	1563	1447	1384	1370	1474	1574	1596						
	1662	1549	-	-	1674	1666	1698	1662	1620	1639	1642	1684	1648	1606	1592	1620	-	1642	1516	1483	1557	1431	1406	1431	1438	1512	1484	1601			
T <sub>1</sub> <b>Qa</b>	1650	1692	-	-	1682	1655	1673	1650	1634	1669	1627	1583	1556	-	1634	1484	1545	1505	1563	1427	1445	1563	1563	1484	1598						
T <sub>1-H</sub> <b>Qa</b>	1650	1703	-	-	1684	1655	1668	1650	1659	1659	1632	1581	1600	1654	1514	1547	1508	1564	1426	1473	1495	1533	1600	1592							
S <sub>0</sub> ' <b>Qa</b>	1638	1711	1707	-	-	1671	1659	1671	1714	1707	1713	1638	1587	1621	1691	1563	1507	1483	1517	1374	1413	1621	1621	1407	1496	1555	1607				
S <sub>0</sub> <b>Qb</b>	1644	-	1684	1366	1689	1676	1665	1717	1674	1669	1644	1578	1578	-	-	1717	1674	1537	1495	1644	1553	1548	1447	1381	1475	1578	1527	1620			
S <sub>1</sub> <b>Qb</b>	1644	1653	-	1685	1366	1690	1679	1644	1674	1596	1669	1644	1574	-	-	1662	1464	1537	1495	1560	1425	1445	1485	1485	1464	1616					
T <sub>1</sub> <b>Qb</b>	1640	1656	-	1685	1365	1653		1670	1640	1656	1629	1644	1672	1629	1676	1656	1574	-	-	1629	1640	1536	1495	1552	1469	1425	1561	1494	1627		
T <sub>1-H</sub> <b>Qb</b>	1640	1655	-	1673	1373	1655	1678	1689	1671	1660	1649	1644	1644	1640	1664	1581	-	1597	1512	1649	1541	1500	1644	1553	1549	1414	1412	1607	1531	1618	
S <sub>0</sub> ' <b>Qb</b>	1643	-	1663	1386	1630	1651	1655	1668	1727	1686	1714	1643	1558	1588	-	1485	1727	1688	1478	1456	1513	1510	1407	1407	1621	1497	1351	1605			
S <sub>0</sub> <b>Qc</b>	1644	1702	-	-	1653	1679	1673	1690	1666	1715	1666	1644	1578	1578	-	1715	1675	1536	1508	1501	1669	1553	1547	1447	1382	1624	1527	1520	1627		
S <sub>1</sub> <b>Qc</b>	1646	1704	-	-	1653	1679	1675	1691	1668	1656	1634	1612	1646	1629	1664	1656	1552	1579	1553	-	1634	1646	1533	1499	1643	1516	1425	1561	1494	1599	SH: 1612
T <sub>1</sub> <b>Qc</b>	1640	1703	-	-	1653	1679	1675	1690	1670	1640	1629	1644	1629	1656	1644	1640	1577	1549	-	1629	1640	1536	1501	1644	1447	1426	1561	1483	1625		
T <sub>1-H</sub> <b>Qc</b>	1649	1652	-	-	1686	1659	1686	1686	1680	1665	1635	1642	1642	1635	1662	1582	1637	1558	1604	1527	1499	1551	1413	1391	1447	1400	1497	1526	1455	1644	
S <sub>0</sub> ' <b>Qc</b>	1644	1643	1654	1661	-	-	1652	1661	1654	1687	1669	1727	1682	1684	1644	1560	1546	1586	1654	1571	1682	1530	1501	1509	1358	1408	1621	1571	1546	1601	
S <sub>0</sub> <b>Qd</b>	1644	-	1681	1387	1655	1678	1674	1687	1665	1716	1675	1645	1644	1575	1644	1669	1555	1578	-	-	1716	1458	1543	1502	1553	1447	1382	1409	1625	1528	1638
S <sub>1</sub> <b>Qd</b>	1652	1655	-	1679	1386	1655	1663	1678	1652	1663	1652	1644	1571	1652	1655	1669	1554	1578	-	-	1663	1679	1544	1502	1561	1454	1404	1369	1483	1463	1632
T <sub>1</sub> <b>Qd</b>	1655	-	1680	1386	1655	1674	1678	1669	1638	1630	1644	1644	1562	1630	1638	1644	1671	1578	-	-	1630	1638	1543	1502	1644	1447	1426	1562	1482	1470	1636
T <sub>1-H</sub> <b>Qd</b>	1639	1655	-	1683	1688	1381	1655	1678	1671	1659	1671	1650	1644	1639	1655	1659	1579	-	1598	1513	1650	1545	1503	1553	1414	1414	1496	1532	1453	1704	
S <sub>0</sub> ' <b>Qd</b>	1641	-	1684	1687	1381	1656	1674	1679	1668	1724	1687	1687	1641	1556	1544	1687	1713	1586	-	1571	1689	1545	1503	1516	1374	1406	1441	1406	1497	1621	
																				1481	1445	1509	1474	1494	1406	1367	1497	1571	1556	1606	

**Table S6** Assignment Tables for major vibrations of the AsLOV2 and RsLOV clusters. Values for the non-deuterated spectra in  $\text{cm}^{-1}$ .

		C=O	C=O	C=N	CHNH	C=O	C=O	C <sub>4</sub> =O <sub>4</sub>	C <sub>2</sub> =O <sub>2</sub>	C=O	C=O	NH <sub>2</sub>	NH <sub>2</sub>	NH <sub>2</sub>	NH <sub>2</sub>	N <sub>5</sub> -H	N <sub>3</sub> -H	N-H	N-H	CH <sub>3</sub>	CH <sub>2</sub>	C-H	O-H	FMN	H <sub>2</sub> O	
AsLOV2	S <sub>0</sub> Qa	1639	1690	-	-	1650 1661 1673 1674 1676 1707	1671 1676	1703	1656	1653 1671 1673	1692	1545	1575 1639	1584	1575 1563	-	1656 1703 1463 1448	1529 1506 1477	1550 1539	1448 1403 1386	1434 1403 1386	1626	-	1575 1626 1532	1602	
	S <sub>1</sub> Qa	1653 1667	1611	-	-	1619 1647 1655 1691	1667	1631	1613	1648 1689	1689	1537 1689	1653	1667	1611	-	1414 1543 1613 1632	1363 1470 1504 1517	1532	1430 1486 1509	1363 1382 1404	1441 1486 1509	-	1486 1509 1537 1594	1598	
	T <sub>1</sub> Qa	1650	1688	-	-	1649 1661 1674 1707	1674 1676	1650	1621	1653 1666	1693	1545	1621 1639 1649	1582	1558	-	1621 1639 1650 1493 1446 1438	1529 1505 1477	1549 1539	1493 1438 1415	1438 1415 1403	1565 1470	-	1565 1493 1470	1605	
	T <sub>1-H</sub> Qa	1641	1698	-	-	1660 1672 1674 1677 1709	1672	1651 1652	1629	1641	1647 1691	1691	1546 1558	1583	1570	1597	1641 1651 1652 1651 1652	1531 1510 1504 1478	1540 1548 1395 1647	1415 1386 1382	1409 1386 1363	1609	-	1534 1597 1609	1598	
	S <sub>0'</sub> Qa	1640 1642	1710 1715	-	-	1672 1674 1702	1679	1710 1715	1670	1689	1698	1537 1550	1559 1640 1642	1579 1581	1545	1581	1670 1499	1531 1501 1482	1646 1509	1526 1487	1435 1424 1381	1425 1409 1383	1621 1494	-	1581 1621	1610
	S <sub>0</sub> Qb	1640	-	1682 1683	1366	1647 1666 1671 1682 1710	1667	1722	1654	1648 1676	1692	1531 1544	1562 1569 1576	1562 1569	-	-	1531 1654 1455 1444	1528 1515 1488 1476	1540 1548	1476 1444 1425 1425	1438 1385 1383 1383	1625 1476	-	1531 1576 1625 1521	1598	
	S <sub>1</sub> Qb	1641	-	1687	1368	1706 1672 1653	1599	1649	1615	1691 1644	1691	1534	1641 1615 1593 1557	1649 1599 1593 1587	-	-	1649 1615 1495	1504 1499 1373	1543 1539	1356	1417 1395 1392 1381	1593 1503 1483	-	1593 1534 1503 1483	1604	
	T <sub>1</sub> Qb	1640 1654	-	1684	1366	1648 1666 1671 1682 1710	1669	1640 1654	1624	1648 1670	1693	1547	1624 1640 1654	1562	-	-	1624 1640 1654 1444 1435	1515 1528 1488 1476	1540 1548	1493 1468 1426 1416	1444 1426 1379	1562 1468	-	1562 1493 1485	1601	
	T <sub>1-H</sub> Qb	1644	-	1675	1358 1367	1649 1666 1671 1683 1711	1659 1673	1659 1673	1629	1646 1676	1691	1540	1562 1572 1629 1644 1649	1562 1572	-	1596	1629 1644 1659 1488 1454	1528 1514 1514 1477	1541 1546	1454 1416 1385 1383	1392 1383 1363	1607 1454	-	1530 1596 1607	1591	
	S <sub>0'</sub> Qb	1643	-	1657	1381 1382	1640 1664 1673 1679	1677 1679 1704	1728	1667	1687 1703	1698	1538 1548	1561 1643	1585	-	1505	1629 1644 1659 1488 1454	1518 1667 1667 1477	1523 1487 1487 1478	1436 1436	1436 1408 1381	1436 1408 1375	1622	-	1548 1622	1603
	S <sub>0</sub> Qc	1651	1697	-	-	1646 1666 1671 1678 1709	1667 1690	1718	1638	1647 1677	1690	1552 1562	1569 1574 1638 1651	1562 1569	-	1638 1651 1458 1445	1514 1522 1493 1475	1526 1548	1445 1390	1390 1387 1386 1379	1627	-	1531 1569 1627 1514	1596		
	S <sub>1</sub> Qc	1643	1697	-	-	1647 1665 1671 1678 1708	1660 1664 1675	1660 1675	1611	1646 1660 1664	1691	1547 1569	1569 1611 1643	1558	-	1611 1660 1675	1512 1520 1493	1512	1399 1520	1381 1377 1361	1574 1486 1399	-	1574 1486 1399	1594		
	T <sub>1</sub> Qc	1647 1655	1698	-	-	1647 1665 1671 1678 1708	1670	1642 1655	1620	1647 1674	1691	1551 1561	1561 1571 1620 1642 1647 1655	1561 1571	-	1620 1642 1446 1438	1476 1493 1513 1521	1524	1470 1490 1419	1419 1389 1382	1470 1490 1375	-	1470 1490 1564	1596		
	T <sub>1-H</sub> Qc	1644 1649 1659	1693	-	-	1649 1667 1671 1679 1711	1672	1659 1672	1623	1649 1674	1690	1551 1563	1563 1573	1553	-	1514 1623 1592 1459 1366	1476 1492 1492 1672 1524	1518 1524	1415 1366	1387 1376 1366	1459	-	1524 1592 1459	1590		

	S'_Qc	1642	1650	-	-	1656 1663 1675 1679 1685	1674	1728	1664	1685 1705	1697	1538 1547	1562 1642	1579	1562	1503	1459 1664	1478 1502 1518	1488 1525	1368	1407 1391 1363	1621	-	1547 1621	1602	
	S₀ Qd	1639 1652	-	1679 1682	1380	1647 1660 1671 1679 1682 1707	1666	1719	1639 1652	1647 1673	1691	1551 1562	1562 1569 1576 1639 1652	1562 1569 1576	-	-	1652 1459 1447	1494 1515 1526 1478	1531 1533 1549 1363	1447 1386 1370	1438 1396 1386	1629	-	1517 1533 1629 1363	1587	
	S₁ Qd	1642 1651	-	1679	1382	1651 1670 1672 1707	1660 1674	1660 1670	1629	1647 1688	1682	1559	1559 1580 1642	1563 1572 1580	-	-	1629 1422	1537 1549 1563 1495 1478	1546 1563	1489 1370 1363	1438 1424 1397 1383	1482 1365	-	1489 1482 1365	1613	
	S₁ Qd2	1644 1659	-	1677	1380	1650 1661 1671 1682 1706	1671	1644 1659 1671	1610	1646 1673	1679	1534 1543 1560	1543 1572 1610 1644 1659	1560 1572	-	-	1543 1610 1644 1671 1362	1501 1532 1534 1525 1429	1504 1534 1534 1646 1437	1378 1381 1389 1398 1378	1478 1504 1587 1362 1362	-	1478 1504 1534 1587 1362	1601		
	T₁ Qd	1655	-	1678 1681	1380	1649 1660 1671 1678 1681 1707	1669	1655	1622	1647 1666	1692	1549	1622 1641 1641 1655	1563	-	-	1622 1641 1655 1515 1438 1447	1478 1495 1515 1526	1545 1549	1467 1402 1419 1427	1369 1373 1379 1396 1438	1467 1485 1563	-	1467 1485 1563	1594	
	T₁-H Qd	1643 1658	-	1685	1380	1649 1660 1671 1680 1707	1673	1658 1673	1627	1649 1674	1691	1541 1560	1560 1570 1627 1643 1658	1560	-	1513 1592 1366	1627 1643 1658 1673 1421	1513 1526 1525 1495	1517 1525 1543	1366 1379 1384 1392	1458	-	1525 1592 1458	1589		
	S₀ Qd	1641 1643	-	1696	1383	1663 1672 1674 1704	1679	1728	1668	1687 1705	1697	1539 1549	1561 1641 1643	1576	-	1500 1379 1668	1500 1503 1516 1479	1525 1367 1379 1406	1375 1379 1380 1406	1622	-	1500 1549 1622	1609			
RsLOV	S₀ Qa	1656	1670 1674	-	-	1649 1687 1693 1700 1711 1721	1693	1719	1663	1669 1683	1708	1573	1538 1552 1656	1586	1577 1583	-	1663 1719 1442 1456	1497 1498 1515 1518 1478	1544 1550	1367 1388 1366 1388	1399 1423 1649	1538 1626	1593			
	S₁ Qa	1671	1649 1656	-	-	1680 1688 1695 1702 1713 1722	1688 1695	1649 1653	1621	1663 1690	1687	1621	1549 1593 1621 1671	1584	1569 1649 1656	-	1621 1649 1653 1387	1496 1499 1517 1482 1485	1541 1545	1510 1364 1371 1416	1510 1420 1656	1510 1545 1592 1364	1617			
	T₁ Qa	1664 1667	1666	-	-	1648 1675 1700 1712 1722	1687 1694	1646	1629	1667 1687	1709	1573	1629 1664	1586	1575 1666	-	1629 1646 1489	1479 1496 1498 1515 1519	1542 1551	1387 1421 1450 1473	1365 1371 1387	1567 1450 1473 1489	1567 1387 1450 1473	1594		
	T₁-H Qa	1658 1672 1673	1691	-	-	1647 1652 1714 1728	1694	1672 1673 1685	1637	1663 1685	1707	1553	1553 1637 1658 1672 1673	1581 1637	1581 1597	1637 1658 1673 1522 1477	1477 1501 1658 1673 1425	1539 1551	1418	1367 1396	1512 1611	1403 1428 1647	1512 1539 1597 1611	1596		
	S₀ Qa	1656	1688	-	-	1649 1654 1668 1686 1694 1713 1730	1694 1686	1737	1674	1706 1727	1714	1569 1562	1547 1562 1656	1591	1578 1359	1579 1674	1501 1505 1523 1476	1512 1483	1359	1368 1369 1380 1416	1623	1401 1649	1562 1579 1623	1596		
	S₀ Qb	1650 1665	-	1691 1698	1362	1658 1676 1679 1691 1705 1711	1689	1737	1650 1665	1668 1689	1707	1575	1555 1567 1581 1650 1665	1555 1567 1581 1650 1665	-	-	1650 1737 1449 1462	1497 1505 1511 1477	1537 1542 1548	1385 1403 1449	1367 1454	1624 1385 1393	1537 1581 1624 1385	1596		
	S₁ Qb	1665 1678 1684	-	1691 1697 1698	1364	1659 1676 1684 1691 1705 1711	1698 1697 1684 1691 1665 1698	1665 1684 1697 1665 1698	1621	1605 1727	1689	1551 1569 1584 1621 1665 1678	1551 1569 1584 1621 1665 1678	1551 1569 1584 1621 1665 1678	-	-	1551 1621 1697 1518 1454 1476	1499 1506 1512 1698	1526 1437	1433 1382 1394	1368 1370 1382 1394	1508 1588 1359 1444 1479	1659 1394	1508 1538 1588 1444 1479	1605 1613	1605
	T₁ Qb	1665 1668	-	1675 1691 1697	1351 1363	1656 1675 1678 1680 1690 1691 1705 1712	1690	1649	1629	1665 1678 1680 1690 1691 1705 1712	1708	1568	1555 1568 1562 1568	1555 1568 1562 1568	-	-	1451 1483 1477 1629 1649 1440	1497 1454 1477 1629 1649 1506	1540 1550	1471 1384 1402	1366 1380	1451 1471 1562	1394 1656	1451 1471 1483 1562 1384	1597	

	T <sub>1-H</sub> Qb	1665 1678	-	1661	1434	1655 1676 1690 1706 1708 1712	1698	1678 1690 1698	1632	1662 1687	1706	1557	1557 1632 1665 1678	1595	-	1532 1542 1603	1632 1698 1414 1434 1459	1479 1490 1496 1516 1517	1541 1542 1549	1414 1418 1434 1459	1368 1378 1396 1403	1459	1397 1655	1532 1603	1596	
	S'_0 Qb	1657	-	1668 1675	1372	1668 1683 1686 1697 1707 1708	1693	1743	1673	1705 1725	1715	1550 1562 1657	1589	-	1622 1369 1380	1673 1459	1475 1482 1497 1511 1513 1528 1452	1507	1362 1369	1370 1380	1622	1668 1398	1562 1622	1598		
	S <sub>0</sub> Qc	1664 1651	1705	-	-	1652 1673 1678 1695 1713	1687	1733	1651 1664	1668 1684	1707	1574 1580	1553 1580 1651 1664	1559	-	1651	1477 1495 1503 1509 1514	1537 1542 1548	1385 1404	1366 1367	1624	1652 1393 1413	1537 1580 1624 1385	1596		
	S <sub>1</sub> Qc	1664 1677	1705	-	-	1654 1674 1681 1690 1696 1713	1664 1694	1681 1694	1621	1606 1727	1689	1569 1621 1664 1677	1569	1558	-	1621 1681 1694	1477 1497 1501 1510 1514 1527	1526 1438	1358 1369 1392 1415	1481 1509 1397 1413	1654 1509	1481 1509 1538	1606 1613			
	T <sub>1</sub> Qc	1665 1667	1705	-	-	1650 1673 1678 1687 1695 1713	1687	1650	1629	1665 1667 1678 1679	1709	1562 1568	1553 1562 1568 1629 1665 1667	1559	-	1450 1495 1503 1629 1511	1450 1472 1385 1550	1450 1366 1379 1401	1450 1472 1483	1650 1414	1472 1483	1597				
	T <sub>1-H</sub> Qc	1658 1671	1703	-	-	1652 1673 1679 1695 1713	1688	1671 1673	1636	1663 1685	1706	1636	1552 1636 1658 1671	1552	1559	1599 1369	1636 1543 1544 1551	1478 1493 1502 1511	1539 1544	1367 1369 1396 1418	1459	1652 1414	1539 1599	1597		
	S'_0 Qc	1655 1660 1670	-	-	-	1682 1694 1703 1712	1690 1694	1733	1674	1705 1726	1714	1549 1560	1549 1560 1655	1579	1567	1359 1378 1413	1674 1492 1506 1516 1531	1475 1488 1492 1506 1516 1531	1483 1510	1359 1378 1413	1366 1369 1413	1623	1425 1398	1560 1623	1597	
	S <sub>0</sub> Qd	1665	-	1650 1654	1434	1654 1680 1687 1694 1703 1707 1713	1687 1694	1736	1651 1665	1669 1683 1687	1707	1575	1556 1582 1651 1665	1573	-	-	1451 1462 1651 1665 1736	1453 1480 1496 1518 1526	1538 1544 1549	1451 1386	1453 1367 1396	1626	1654 1386	1538 1582 1626	1594	
	S <sub>1</sub> Qd	1666	-	1644	1440	1655 1679 1691 1698 1704 1707 1713	1680 1698	1666 1689 1698	1552 1622	1610 1725	1689 1691	1583 1588 1622	1552 1582	1552	-	-	1443 1552 1622 1666 1680 1622 1698	1453 1480 1480 1498	1437 1528	1408 1426 1434	1394 1419	1508 1588	1395 1424 1655	1481 1508 1538 1588	1605	
	T <sub>1</sub> Qd	1665 1668	-	1646	1436	1653 1679 1687 1695 1708 1713	1687 1695	1646 1650 1668	1629	1665 1678	1709	1575	1556 1629 1665 1668	1566	-	-	1451 1483 1629 1646 1650 1438	1453 1480 1496 1497 1517 1528	1542 1550	1451 1471 1384 1404	1366 1380 1384 1428	1451 1471 1483 1566	1395 1423 1653	1451 1471 1483 1566	1596	
	T <sub>1-H</sub> Qd	1661 1676	-	1666 1661	1430	1652 1680 1690 1697 1703 1707 1713	1690 1697	1676 1690 1697	1636	1663 1685	1706	1555	1555 1636 1661 1676	1581	-	1599	1636 1676 1690 1415 1436 1461	1478 1491 1495 1514 1520 1525	1539 1544 1551	1418 1461	1367 1372 1394 1415	1461	1398 1423 1652	1539 1599	1595	
	S'_0 Qd	1656	-	1666	1420	1654 1680 1685 1700 1706 1715	1695	1740	1675	1705 1728	1713	1562 1569	1550 1562 1656	1562	1587	-	1362	1675 1454	1475 1491 1498 1516 1520	1484 1512	1362 1369	1369 1380 1449	1622	1397 1426 1654	1562 1622	1596

**Table S7** Evolution of selected **Qb**, **Qd** EL222 and AsLOV2 IR peaks along the reaction coordinate. Isotopic shifts from the non-deuterated spectra are given with red numbers. Values in  $\text{cm}^{-1}$ .

		<b>S<sub>0</sub></b>	<b>S<sub>1</sub></b>	<b>T<sub>1</sub></b>	<b>T<sub>1-H</sub></b>	<b>S'<sub>0</sub></b>
<b>sC=N</b>	<b>EL222</b>	<b>Qb</b> 1663- <b>21</b> m	1664- <b>21</b> m	1664- <b>21</b> m	1653- <b>20</b> m	1654- <b>9</b> w
	<b>AsLOV2</b>	<b>Qd</b> 1660- <b>21</b> w	1658- <b>20</b> w	1660- <b>20</b> w	1664- <b>19</b> m	1664- <b>20</b> w
	<b>EL222</b>	<b>Qb</b> 1662- <b>20</b> m	1666- <b>21</b> w	1663- <b>21</b> w	1655- <b>20</b> w	1639- <b>18</b> m
	<b>AsLOV2</b>	<b>Qd</b> 1661- <b>18</b> m	1661- <b>18</b> m	1661- <b>17</b> m	1664- <b>21</b> m	1684- <b>11</b> m
<b>sC<sub>2</sub>=O<sub>2</sub></b>	<b>EL222</b>	<b>Qb</b> 1665+ <b>0</b> m, 1674+ <b>0</b> m	1593- <b>3</b> s	1629+ <b>0</b> w	1649+ <b>0</b> vs	1687- <b>1</b> m
	<b>AsLOV2</b>	<b>Qd</b> 1665+ <b>0</b> w, 1675+ <b>0</b> m	1652+ <b>0</b> s	1630+ <b>0</b> w, <i>a</i> -1638+ <b>0</b> vs	1650+ <b>0</b> vs	1688- <b>1</b> s
	<b>EL222</b>	<b>Qb</b> 1654+ <b>0</b> s	1615+ <b>0</b> s	<i>a</i> -1640+ <b>0</b> vs, 1624+ <b>0</b> m	1628- <b>1</b> m	1666- <b>1</b> m, 1677+ <b>0</b> w
	<b>AsLOV2</b>	<b>Qd</b> 1639+ <b>0</b> w, 1652+ <b>0</b> s	1629+ <b>0</b> s	1622+ <b>0</b> m, <i>a</i> -1641+ <b>0</b> s	1627+ <b>0</b> m, <i>a</i> - 1643+ <b>0</b> s	1667- <b>1</b> s, 1679+ <b>0</b> m
<b>sC<sub>4</sub>=O<sub>4</sub></b>	<b>EL222</b>	<b>Qb</b> 1717+ <b>0</b> m	1662+ <b>0</b> m, 1674+ <b>0</b> w	1656+ <b>0</b> w	1672+ <b>1</b> m	1726- <b>1</b> m
	<b>AsLOV2</b>	<b>Qd</b> 1715+ <b>0</b> w	1680- <b>1</b> w	<i>a</i> -1638+ <b>0</b> vs, 1655+ <b>0</b> m	1658- <b>1</b> m	1724+ <b>0</b> w
	<b>EL222</b>	<b>Qb</b> 1722+ <b>0</b> m	1587+ <b>0</b> s, 1649+ <b>0</b> w	<i>a</i> -1640+ <b>0</b> vs, 1654+ <b>0</b> m	1659+ <b>0</b> m, 1673+ <b>0</b> w	1727- <b>1</b> m
	<b>AsLOV2</b>	<b>Qd</b> 1719+ <b>0</b> m	1671+ <b>1</b> s, 1674+ <b>0</b> m	<i>s</i> -1641+ <b>0</b> s, 1655+ <b>0</b> w	<i>a</i> -1643+ <b>0</b> s, 1673+ <b>0</b> w, 1658+ <b>0</b> m	1727- <b>1</b> m
<b>rHINCOH</b>	<b>EL222</b>	<b>Qb</b> 1259- <b>107</b> w	1259- <b>107</b> w	1259- <b>106</b> w	1266- <b>107</b> w	1257- <b>129</b> w
	<b>AsLOV2</b>	<b>Qd</b> 1241- <b>146</b> w	1242- <b>144</b> w	1242- <b>144</b> w	1230- <b>151</b> w	1233- <b>148</b> w
	<b>EL222</b>	<b>Qb</b> 1258- <b>100</b> vw, 1264- <b>102</b> w	1224- <b>134</b> w,	1256- <b>102</b> vw, 1263- <b>103</b> w	1260- <b>98</b> vw, 1265- <b>102</b> w	1277- <b>105</b> vw
	<b>AsLOV2</b>	<b>Qd</b> 1238- <b>142</b> w	1239- <b>142</b> w	1239- <b>141</b> w	1227- <b>153</b> w	1206- <b>177</b> w

Intensities vs: very strong, s: strong, m: medium, w: weak, vw: very weak

Assignments: *s*: stretch, *a*: antisymmetric, *s*: symmetric, *r*: rocking, *sc*: scissor

**Table S8** Evolution of selected RsLOV IR peaks along the reaction coordinate. Underlining denotes that *scNH<sub>2</sub>/rHNCOH*, or *rOH* are major modes in that vibration. Isotopic shifts from the non-deuterated spectra are given with red numbers – with the exception of the *scNH<sub>2</sub>/rHNCOH*, and *rOH* modes that shift below 1350 cm<sup>-1</sup> in D<sub>2</sub>O. All values in cm<sup>-1</sup>.

	S <sub>0</sub>	S <sub>1</sub>	T <sub>1</sub>	T <sub>1-H</sub>	S' <sub>0</sub>
<i>sC=O/sC=N</i>	<b>Qa</b> 1659- <u>11</u> w, 1664- <u>10</u> m	1636- <u>13</u> s, 1652- <u>4</u> w	1656+ <u>10</u> s, 1666 w 1667- <u>8</u> w, 1682- <u>9</u> w, 1697 w	1681- <u>10</u> m, 1685- <u>9</u> w 1641- <u>20</u> m	1679- <u>9</u> m 1658- <u>9</u> m, 1669- <u>6</u> w 1684- <u>2</u> m
	<b>Qb</b> 1668- <u>8</u> w, 1682- <u>16</u> m	1668- <u>29</u> w, 1682- <u>16</u> m			
	<b>Qc</b> 1700- <u>5</u> m	1700- <u>5</u> m	1700- <u>5</u> m	1699- <u>3</u> m	1646- <u>14</u> w, 1668- <u>2</u> s
	<b>Qd</b> 1635- <u>19</u> m	1628- <u>16</u> w	1633- <u>13</u> s, 1650 m	1643- <u>18</u> vs, 1649- <u>17</u> w	1645- <u>21</u> m
<i>sC<sub>2</sub>=O<sub>2</sub></i>	<b>Qa</b> 1664- <u>1</u> vs	1621+ <u>0</u> s	s-1629+ <u>0</u> m <i>a</i> -1645- <u>1</u> vs	1636- <u>1</u> s	1674+ <u>0</u> vs
	<b>Qb</b> 1650+ <u>0</u> w, 1665- <u>1</u> vs	1621+ <u>0</u> vs	s-1629+ <u>0</u> m, <i>a</i> -1649+ <u>0</u> s	1631- <u>1</u> s	1673+ <u>0</u> vs, 1693+ <u>0</u> w
	<b>Qc</b> 1651+ <u>0</u> w, 1664+ <u>0</u> vs	1621+ <u>0</u> vs	s-1629+ <u>0</u> m, <i>a</i> -1650+ <u>0</u> s	s-1636+ <u>0</u> m, <i>a</i> -1658+ <u>0</u> vs	1674+ <u>0</u> vs
	<b>Qd</b> 1651+ <u>0</u> w, 1665+ <u>0</u> vs	1622+ <u>0</u> vs	s-1629+ <u>0</u> m, <i>a</i> -1648+ <u>2</u> s	s-1635- <u>1</u> m, <i>a</i> -1662+ <u>1</u> vs	1676+ <u>1</u> vs
<i>sC<sub>4</sub>=O<sub>4'</sub></i>	<b>Qa</b> 1718- <u>1</u> w	1652- <u>1</u> m	1665- <u>2</u> , <i>a</i> -1645- <u>1</u> s, <i>s</i> -1629+ <u>0</u> m	1672+ <u>0</u> m, 1685+ <u>0</u> m	1737+ <u>0</u> w
	<b>Qb</b> 1737+ <u>0</u> w	1684+ <u>0</u> w, 1698+ <u>0</u> m	s-1629+ <u>0</u> m, <i>a</i> -1649+ <u>0</u> s, 1667- <u>1</u> w	1677+ <u>0</u> m, 1690+ <u>0</u> w, 1698+ <u>0</u> w	1742- <u>1</u> w
	<b>Qc</b> 1733+ <u>0</u> w	1664+ <u>0</u> vs, 1693- <u>1</u> w	s-1629+ <u>0</u> m, <i>a</i> -1650+ <u>0</u> s, 1666- <u>1</u> w	s-1636+ <u>0</u> m, <i>a</i> -1658+ <u>0</u> vs, 1671+ <u>0</u> w, 1678- <u>1</u> w	1733+ <u>0</u> w
	<b>Qd</b> 1736+ <u>0</u> w	1666+ <u>0</u> vs, 1680+ <u>0</u> w, 1697- <u>1</u> m	s-1629+ <u>0</u> m, <i>a</i> -1648+ <u>2</u> s, 1649- <u>1</u> m, 1667+ <u>0</u> w	s-1635- <u>1</u> m, <i>a</i> -1662+ <u>1</u> vs, 1676+ <u>0</u> m, 1689- <u>1</u> w	1739+ <u>4</u> w
<i>scNH<sub>2</sub>/rHNCOH</i>	<b>Qa</b> 1577 w, <u>1583</u> s	1569 vw	1567 m, <u>1575</u> vv	<u>1579</u> vw, 1581 w	<u>1578</u> w, 1579 vw
	<b>Qb</b> 1362 w	1364 vw	1363 w	1403 w	1372 w
	<b>Qc</b> <u>1559</u> w	<u>1558</u> w	1559 w	1559 w	1567 w
	<b>Qd</b> <u>1434</u> vw	<u>1440</u> vw	<u>1436</u> vv	<u>1430</u> vv	<u>1420</u> vw
<i>rOH</i>	<b>Qa</b> 1399 w, 1649 m	1420 vw, 1656 w	1399 w, 1424 vw, 1648 m	1402 w, 1428 w, 1647 m 1399 vv, 1425 vv, 1655 m	1401 w, 1426 vw, 1649 m 1372 w, 1398 vv, 1668 w
	<b>Qb</b> 1658 w	1394 w, 1421 vv, 1659 w	1394 w, 1421 vv, 1656 w		
	<b>Qc</b> 1413 w, 1652 w	1413 w, 1654 w	1414 vw, 1650 w	1414 w, 1652 w	<u>1398</u> vw, 1427 vv
	<b>Qd</b> 1424 vw, 1654 m	1395 vw, 1655 m	1395 w, 1653 w	1398 w, 1652 w	1397 w, 1654 w

Intensities vs: very strong, s: strong, m: medium, w: weak, vw: very weak

Assignments: s: stretch, *a*: antisymmetric, *s*: symmetric, *r*: rocking, *sc*: scissor

## 2b. Difference Spectra

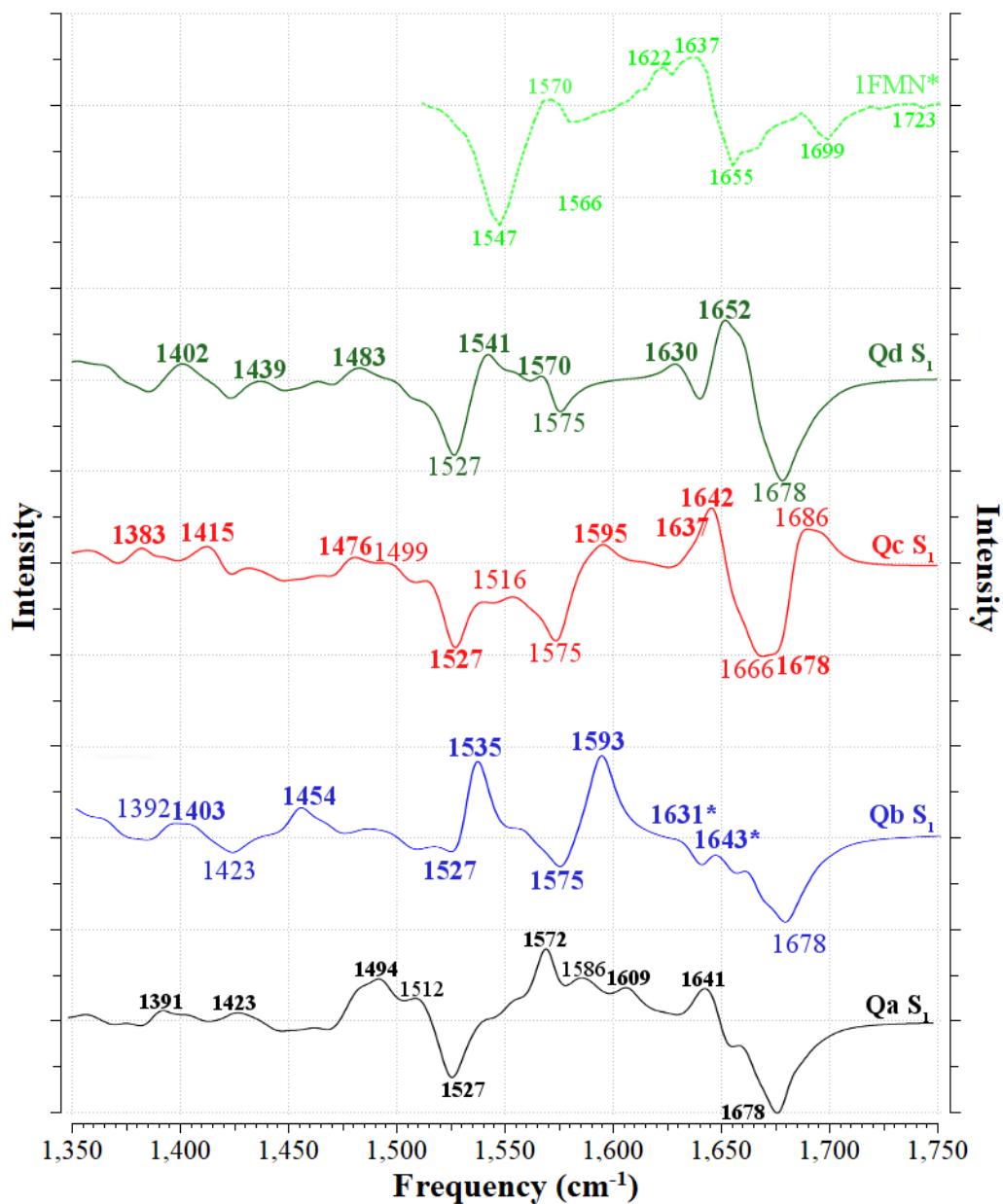


Figure S23 Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the  $S_1$  states of **Qa-Qd** of the EL222 cluster. The difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), and **Qd** (—) are included with the indicated line colours. The experimental 1FMN\* EADS of EL222 is included in light green (—). The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-maximum peak (HWHM) of  $8\text{ cm}^{-1}$  was applied to resemble the experimental curve. The apparent strongest peaks after subtraction are labelled with the respective colour.

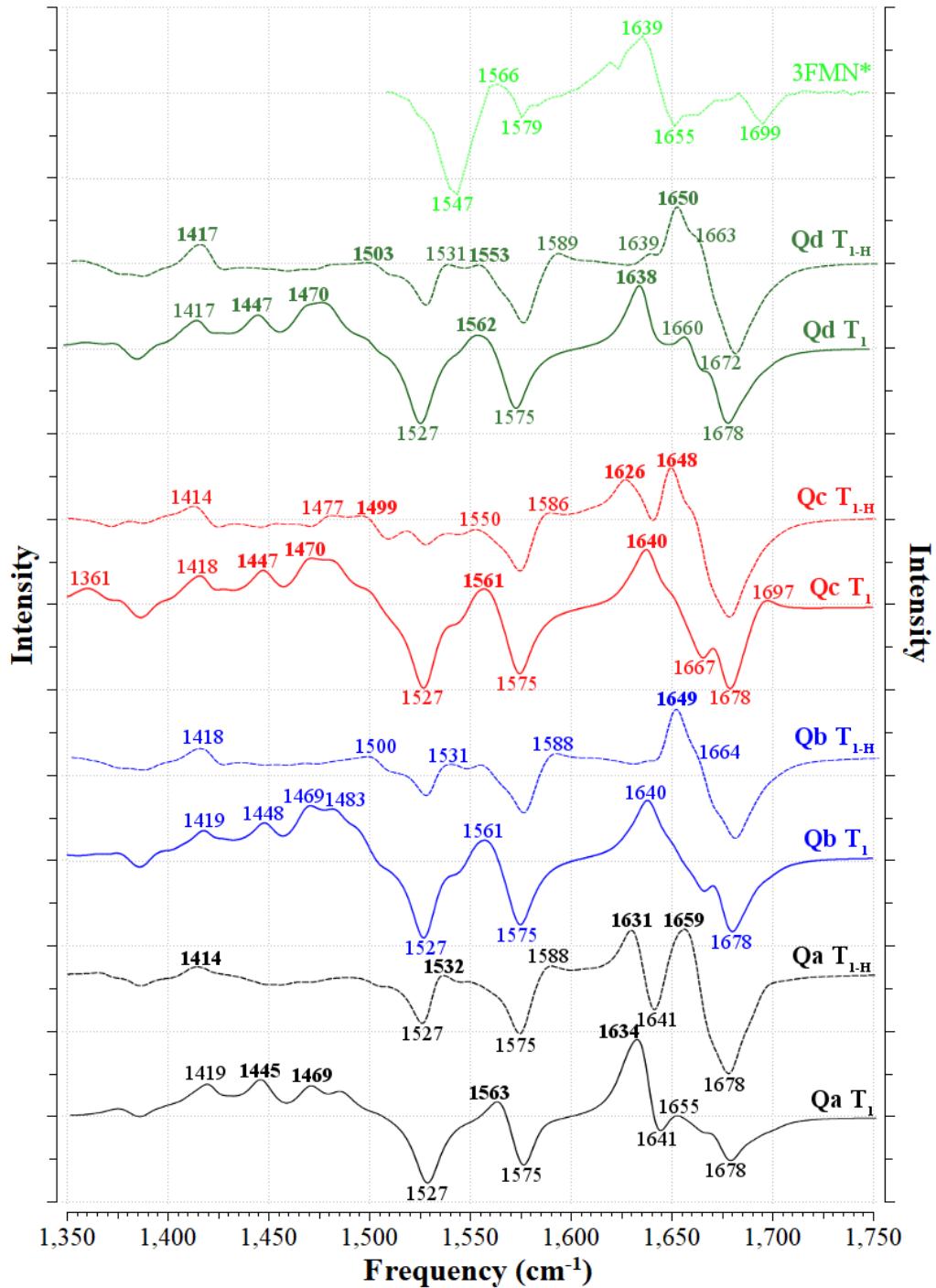


Figure S24 Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the  $T_1$  and  $T_{1-H}$  states of **Qa-Qd** of the EL222 cluster. The  $T_1$  difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), **Qd** (—) and the  $T_{1-H}$  difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), and **Qd** (—) are plotted with the indicated line colours. The experimental 3FMN\* EAS spectrum of EL222 is included in light green (—). The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-maximum peak (HWHM) of  $8 \text{ cm}^{-1}$  was applied to resemble the experimental curve. The apparent strongest peaks after subtraction are labelled with the respective colour.

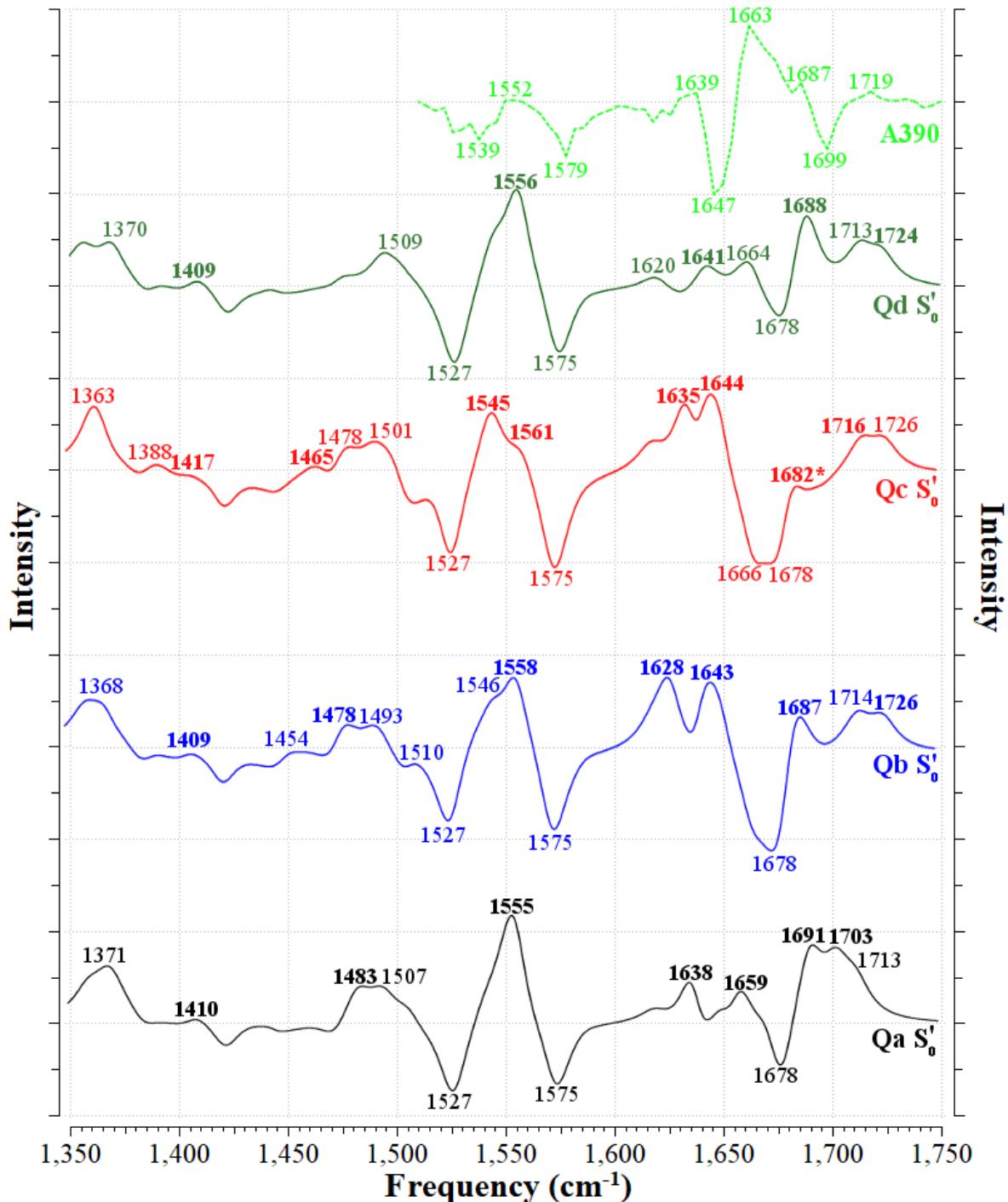
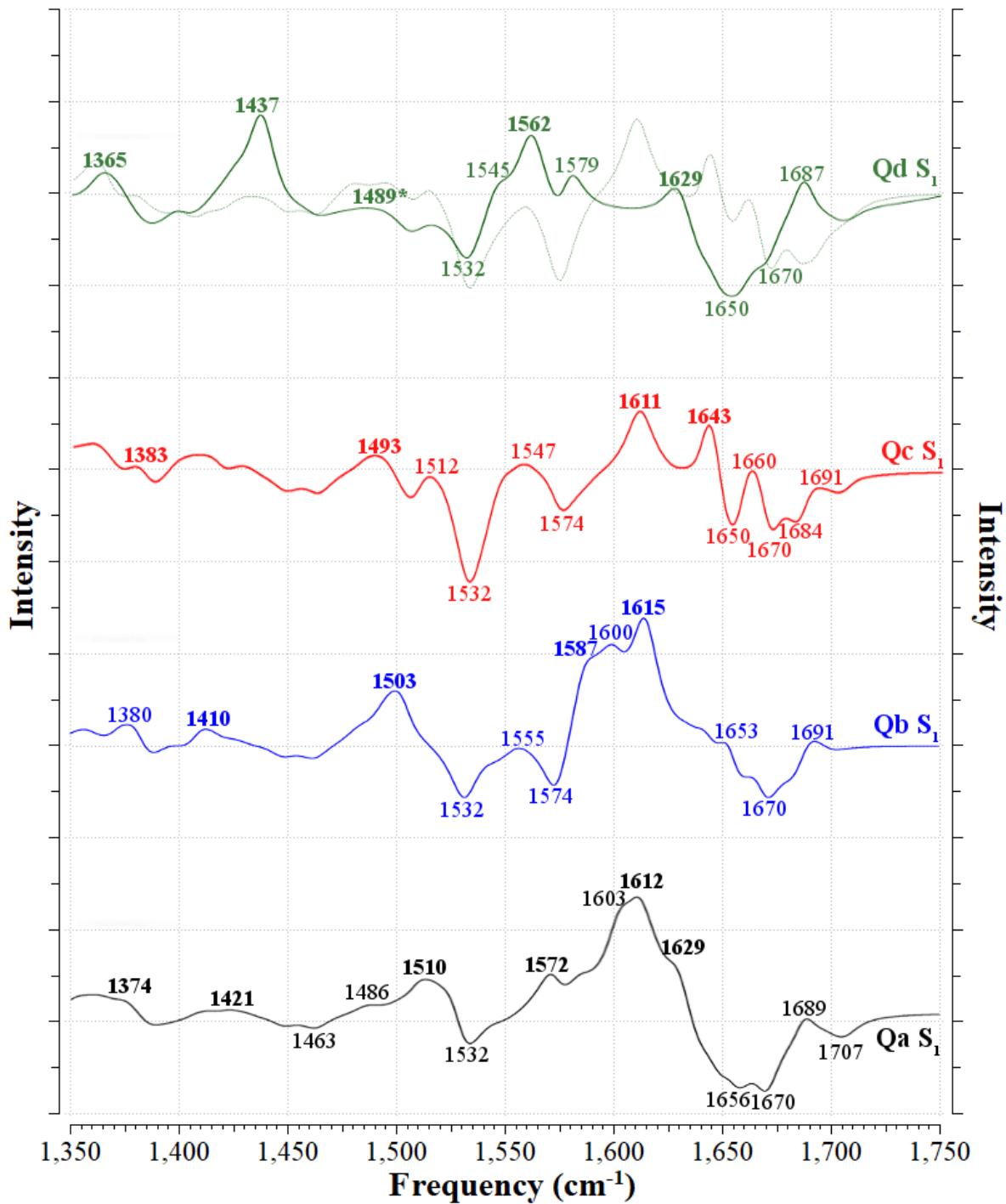
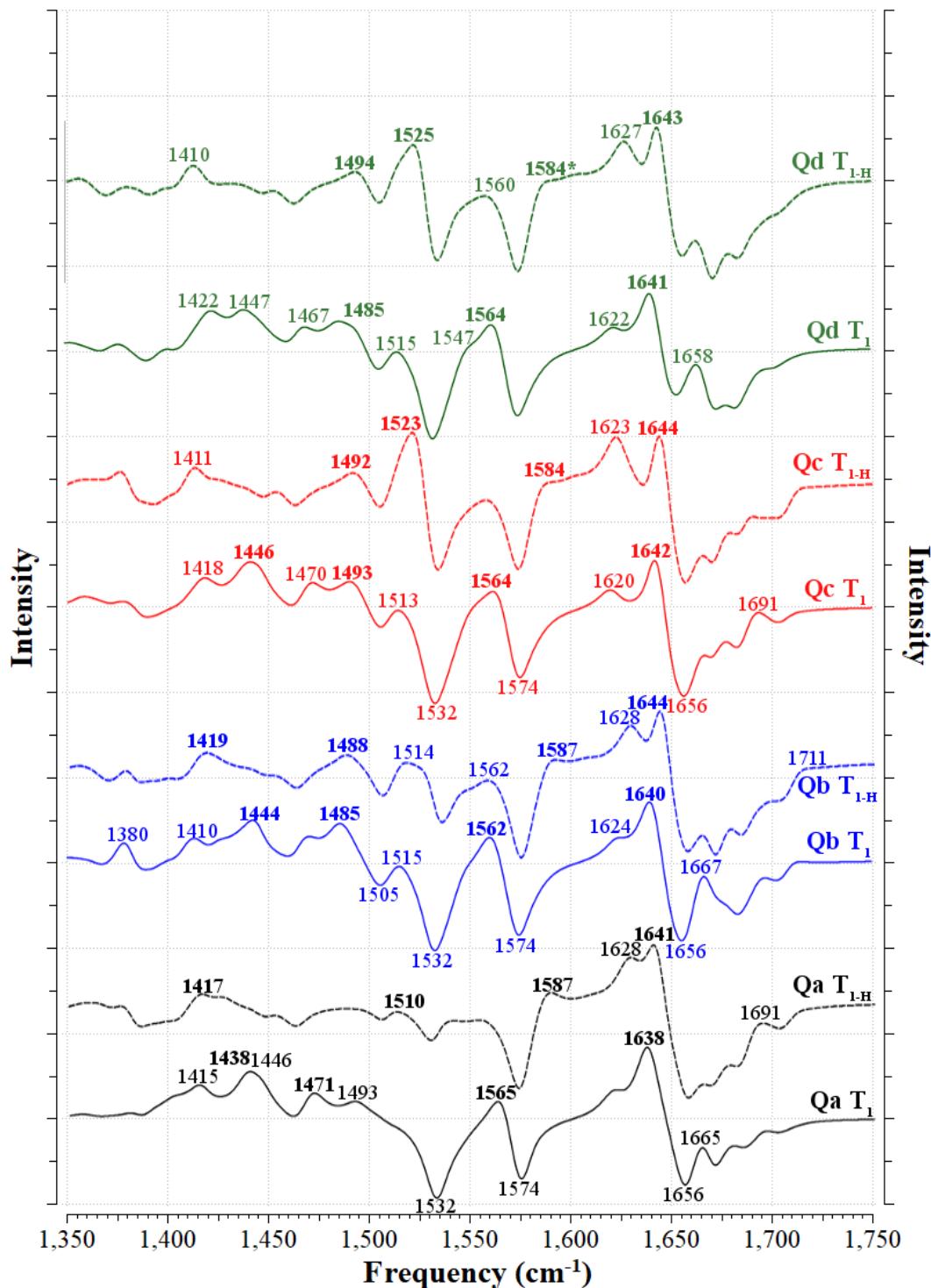


Figure S25 Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the adduct  $S'_0$  states of **Qa-Qd** of the EL222 cluster. The difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), and **Qd** (—) are plotted with the indicated line colours. The experimental A390 EADS of EL222 is included in light green (—). The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-maximum peak (HWHM) of 8 cm<sup>-1</sup> was applied to resemble the experimental curve. The apparent strongest peaks after subtraction are labelled with the respective colour.



**Figure S26** Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the  $S_1$  states of **Qa-Qd** of the AsLOV2 cluster. The difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), **Qd** (—) and **Qd'** (—) are plotted with the indicated line colours. The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$  was applied to resemble the experimental curve. The apparent strongest peaks after subtraction are labelled with the respective colour.



**Figure S27** Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the  $T_1$  and  $T_{1-H}$  states of **Qa-Qd** of the AsLOV2 cluster. The  $T_1$  difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), **Qd** (—) and the  $T_{1-H}$  difference spectra of **Qa** (---), **Qb** (—), **Qc** (—), and **Qd** (—) are included with the indicated line colours. The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$  was applied to resemble the experimental curve. The apparent strongest peaks after subtraction are labelled with the respective colour.

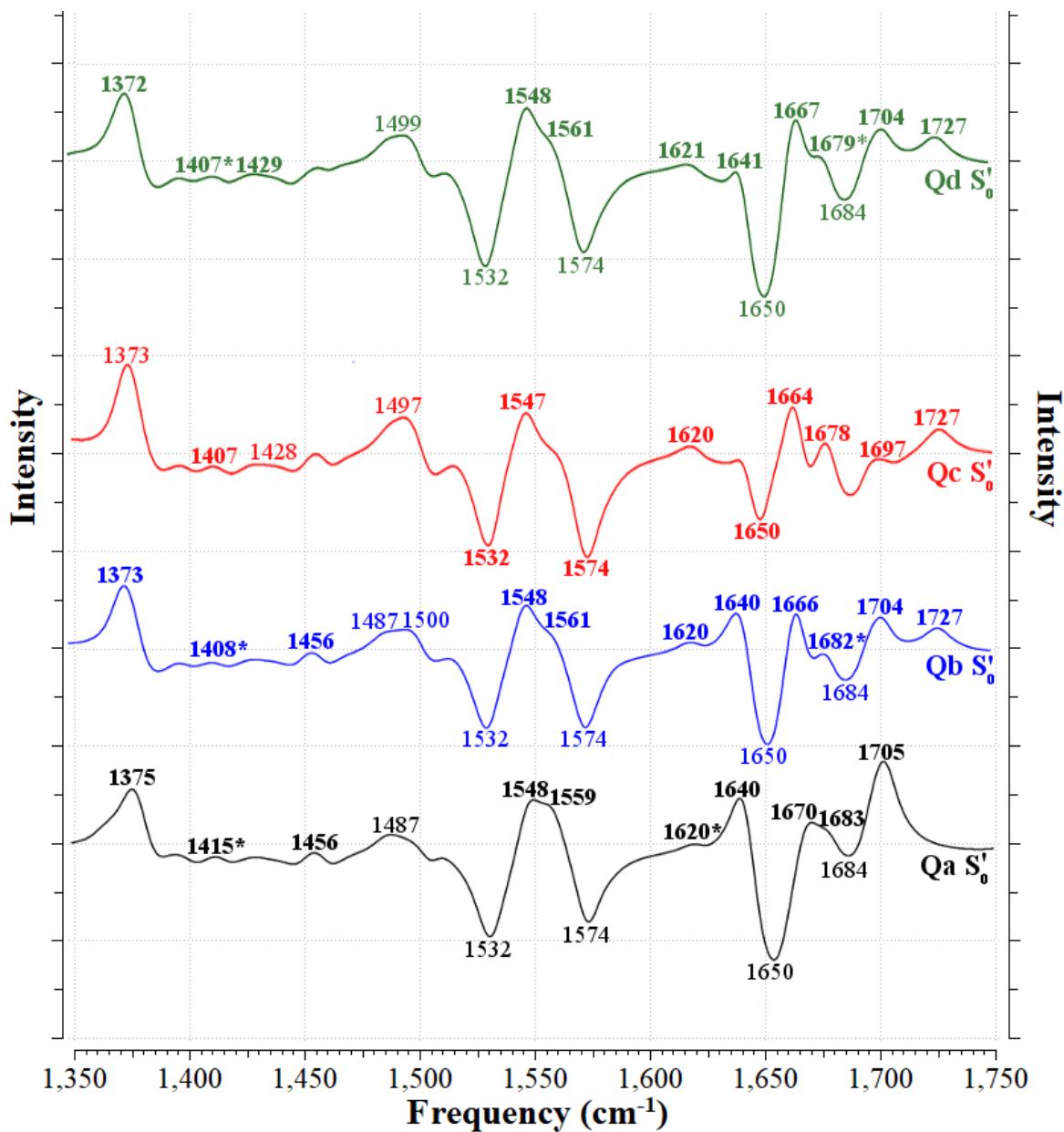
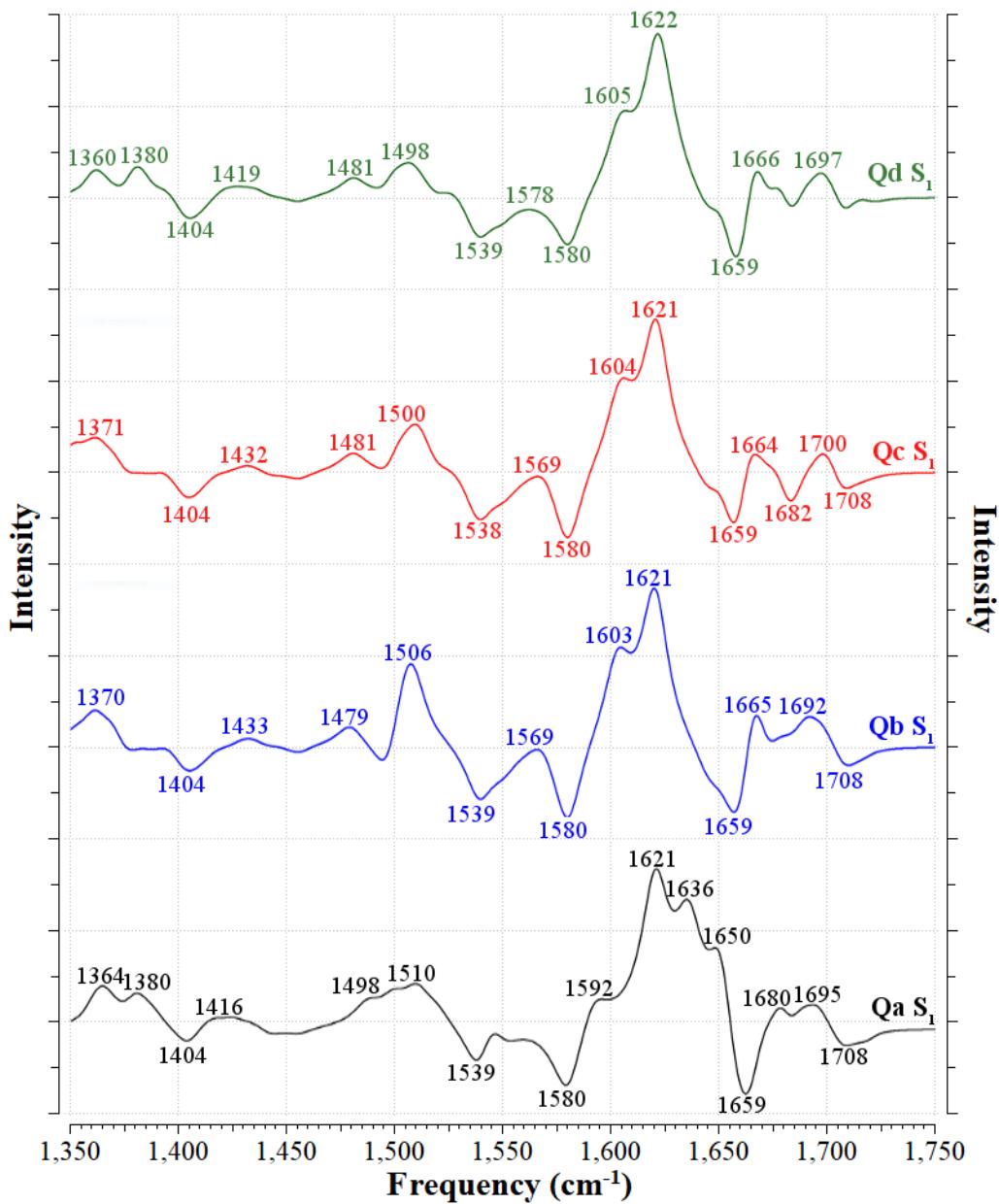
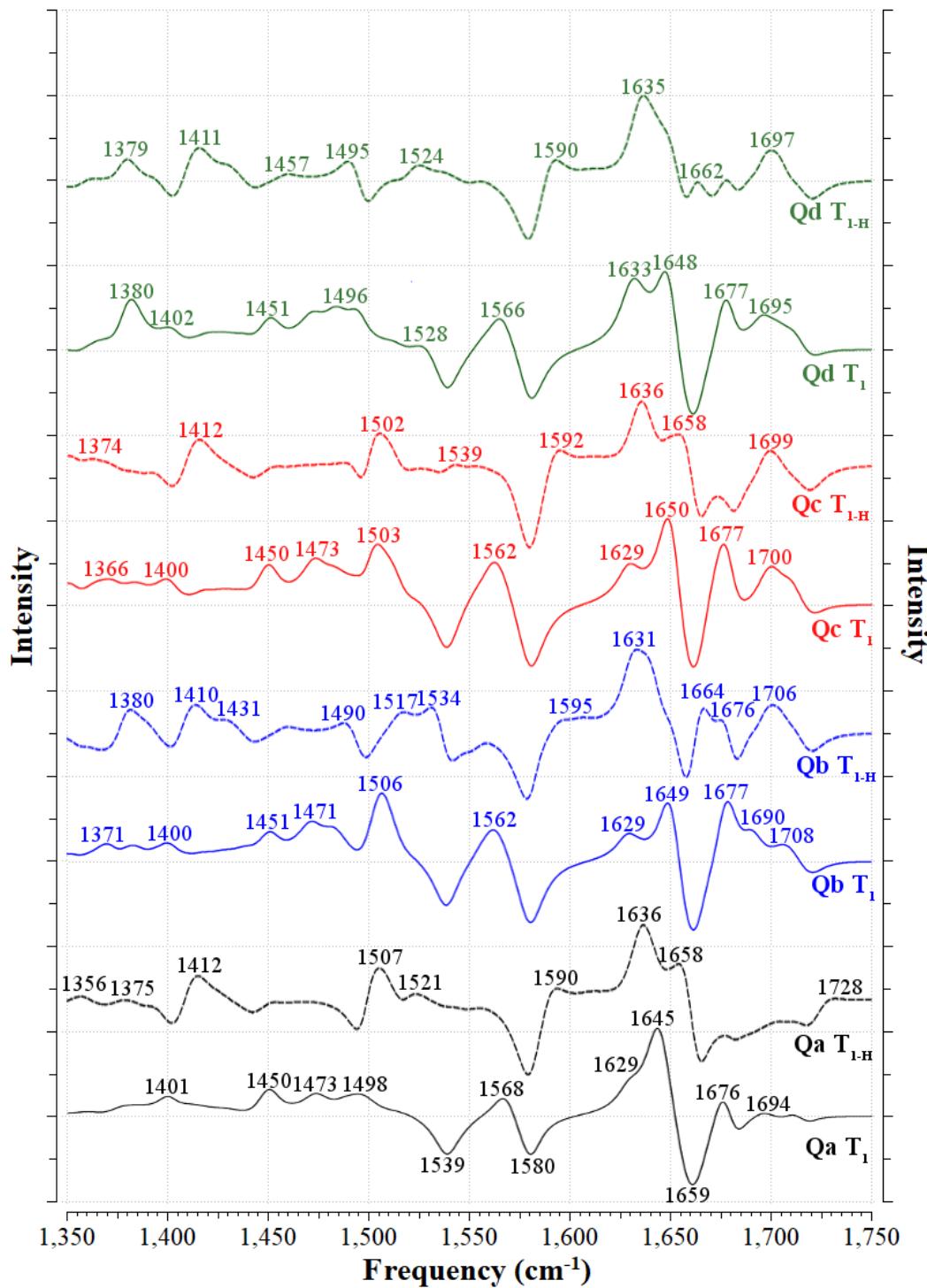


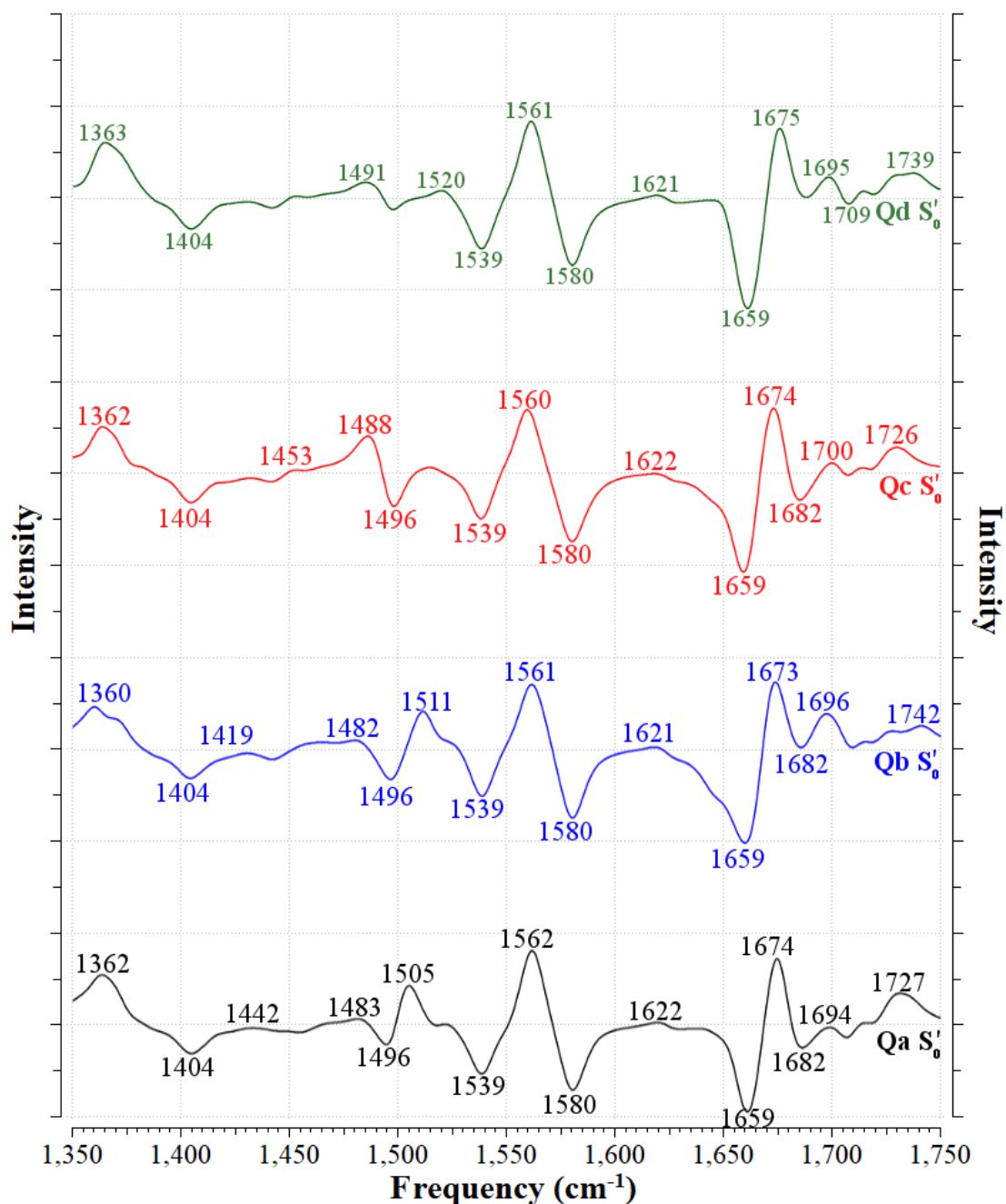
Figure S28 Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the adduct  $S_0'$  states of **Qa-Qd** of the AsLOV2 cluster. The difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), and **Qd** (—) are included with the indicated line colours. The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-height maximum (HWHM) of 8 cm<sup>-1</sup> was applied to resemble the experimental curve. The apparent strongest peaks after subtraction are labelled with the respective colour.



**Figure S29** Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the  $S_1$  states of **Qa-Qd** of the RsLOV cluster. The difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), and **Qd** (—) are included with the indicated line colours. The spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-height maximum (HWHM) of 8 cm<sup>-1</sup> was applied. The apparent strongest peaks after subtraction are labelled with the respective colour. Since the same  $S_0$  spectrum is subtracted from all plots, the negative peaks ground state peaks are labelled mostly in the first **Qa** (—) plot.



**Figure S30** Calculated deuterated infrared difference spectra between the ground state  $S_0$  of **Qa** and the  $T_1$  and  $T_{1-H}$  states of **Qa-Qd** of the RsLOV cluster. The  $T_1$  difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), **Qd** (—) and the  $T_{1-H}$  difference spectra of **Qa** (---), **Qb** (—), **Qc** (—), and **Qd** (—) are included with the indicated line colours. The spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$  was applied. The apparent strongest peaks after subtraction are labelled with the respective colour. Since the same  $S_0$  spectrum is subtracted from all plots, the negative peaks belonging to the **Qa** ground state are labelled mostly in the first **Qa** (—) plot.



**Figure S31** Calculated deuterated infrared difference spectra between the ground state of **Qa** and the adduct  $S'_0$  states of **Qa-Qd** of the RsLOV cluster. The difference spectra of **Qa** (—), **Qb** (—), **Qc** (—), and **Qd** (—) are included with the indicated line colours. The calculated spectra were normalised before subtraction, scaled by 0.97 and a half-width at half-height maximum (HWHM) of  $8 \text{ cm}^{-1}$  was applied. The apparent strongest peaks after subtraction are labelled with the respective colour. Since the same  $S_0$  spectrum is subtracted from all plots, the negative peaks ground state peaks are labelled mostly in the first **Qa** (—) plot.

**Table S9** EL222 and AsLOV2 IR spectra assignments for the **Qa** and **Qc** models. Normal modes are coloured according to residue; FMN black, Q138/Q513 red, C75/C450 orange, N107/N482 green, N117/N492 violet, Q454 grey, A39/N414 blue and other backbone modes, light blue. Mean absolute deviations are included for each theoretical/experimental correlation. Isotopic shifts from the non-deuterated spectra are given with red numbers. All values in  $\text{cm}^{-1}$ .

### EL222

Exp.	Qa	Assignment	Qc	Assignment
<b>1FMN*</b> <b>Ground State (<math>S_0</math>)</b>				
1547 <sup>†</sup>	1527+0	FMN	1527+0	FMN
1579 <sup>†</sup>	1575+1	FMN, scNH <sub>2</sub>	1574+0	FMN, scNH <sub>2</sub>
1655 <sup>†</sup>	1667-1	sC=O, sC <sub>2</sub> =O <sub>2</sub>	1669+0	sC=O, sC <sub>2</sub> =O <sub>2</sub>
1699 <sup>†</sup>	1688-5	sC=O, sC <sub>4</sub> =O <sub>4</sub>	1695-7	sC=O, sC <sub>4</sub> =O <sub>4</sub>
MAD	11.8 (11.0)		10.8 (10.5)	
<b>1FMN*</b> <b>Excited State (<math>S_1</math>)</b>				
1378 <sup>‡</sup>	1391+1	rN <sub>3</sub> -H, CH <sub>3</sub>	1383-1	FMN, rN <sub>3</sub> -H
1419 <sup>‡</sup>	1423+17	CH <sub>3</sub> , rN <sub>3</sub> -H, CH <sub>2</sub>	1415+1	scCH <sub>2</sub> , CH <sub>3</sub> /sC-N
1498 <sup>‡</sup>	1494+2 <i>rN-H</i>	1512+0 FMN, scCH <sub>2</sub> , CH <sub>3</sub>	1476+0 <i>rN-H</i>	
1571 <sup>†</sup>	1572-34	scNH <sub>2</sub> , sC=O (scNH <sub>2</sub> )	1595-4	sC=O/FMN, rC <sub>6,9</sub> -H, sH <sub>2</sub> O
1623 <sup>†</sup>	1609-11	scNH <sub>2</sub> , sC <sub>2</sub> =O <sub>2</sub> , sC <sub>4</sub> =O <sub>4</sub> ; (scNH <sub>2</sub> )	1637#-6	sC=O, scNH <sub>2</sub>
1639 <sup>†</sup>	1641-1	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , scNH <sub>2</sub>	1642-4	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , scNH <sub>2</sub>
MAD	6.3 (12.0)		12.0 (14.7)	
<b>3FMN*</b> <b>Excited State (<math>T_1</math>)</b>				
1428 <sup>‡</sup>	1445+0	scCH <sub>2</sub> , rN <sub>3</sub> -H, CH <sub>3</sub>	1447+0	rN <sub>3</sub> -H, scCH <sub>2</sub>
1488 <sup>‡</sup>	1469+0	CH <sub>3</sub> , rC <sub>6,9</sub> -H	1470+1	FMN, CH <sub>3</sub>
1567 <sup>†</sup>	1563+0	CH <sub>3</sub> , rC <sub>6,9</sub> -H	1561+0	FMN, scNH <sub>2</sub>
1639 <sup>†</sup>	1634+0	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub>	1640+0	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , sC=O, sC <sub>4</sub> =O <sub>4</sub>
MAD	11.3 (11.3)		11.0 (11.3)	
<b>3FMN*</b> <b>Excited State (<math>T_{1-H}</math>)</b>				
1428 <sup>‡</sup>	1414-1	rN <sub>3</sub> -H, CH <sub>3</sub> , scCH <sub>2</sub>	1412#-1	CH <sub>3</sub> , scCH <sub>2</sub>
1488 <sup>‡</sup>	1508#+0 <i>rN-H</i>		1499#+0 <i>rN-H</i>	
1567 <sup>†</sup>	1532-1	FMN, <i>rN-H</i>	1586-18	FMN, scNH <sub>2</sub> , (rN <sub>5</sub> -H)
1639 <sup>†</sup>	1631-1 <i>rN<sub>3</sub>-H, sC=O, sC<sub>4</sub>=O<sub>4</sub></i>	1659+0 <i>rN<sub>3</sub>-H, sC=O, sC<sub>2</sub>=O<sub>2</sub></i>	1626-11 <i>sC=O (scNH<sub>2</sub>)</i>	
MAD	19.3 (18.5)		14.8 (16.3)	
<b>A390</b> <b>Adduct State (<math>S_0^+</math>)</b>				
-	-	-	-	-
1418 <sup>‡</sup>	1410+3	CH <sub>2</sub> /CH <sub>3</sub> , rN <sub>5</sub> -H	1417+3	scCH <sub>2</sub>
1450 <sup>‡</sup>	1483+0 <i>rN-H</i>		1465+1	rN <sub>3</sub> -H
1555 <sup>†</sup>	1555+0	scNH <sub>2</sub> , FMN	1545-1	scNH <sub>2</sub> , FMN (rN <sub>5</sub> -H)
-	-	-	1561+1	scNH <sub>2</sub> , FMN
1639 <sup>†</sup>	1638+0 <i>sC=O</i>		1635-8 <i>sC=O, sC=O (sC=O)</i>	
1663 <sup>†</sup>	1659-12 <i>sC=O</i>		1644+0 <i>sC=O, scNH<sub>2</sub></i>	
1687 <sup>†</sup>	1691+0 <i>rN<sub>3</sub>-H, sC<sub>2</sub>=O<sub>2</sub></i>		1682#+0 <i>sC<sub>2</sub>=O<sub>2</sub>, rN<sub>3</sub>-H</i>	
-	-	-	-	-
1719 <sup>†</sup>	1703-4 <i>sC<sub>2</sub>=O<sub>2</sub>, sC=O, sC<sub>4</sub>=O<sub>4</sub></i>		1716+0 <i>sC=O</i>	
1713+0 <i>sC=O</i>			1726-1 <i>sC<sub>4</sub>=O<sub>4</sub>, rN<sub>3</sub>-H (rN<sub>5</sub>-H)</i>	
MAD	8.0 (9.0)		7.6 (7.7)	

FMN: ring breathing, *r*: rocking, *s*: stretch, *sc*: scissoring

#: Relatively intense ES peak in proximity to the experimental, offset by the GS signal

(): Normal mode only in non-deuterated spectrum

†: This study

‡: Taken from ref.<sup>32</sup>

### AsLOV2

Exp.	Qa	Assignment	Qc	Assignment
<b>1FMN*</b> <b>Ground State (<math>S_0</math>)</b>				
1550 <sup>‡</sup>	1532+0	FMN, rN <sub>3</sub> -H, scNH <sub>2</sub>	1531+0	FMN, rN <sub>3</sub> -H, scNH <sub>2</sub>
1583 <sup>‡</sup>	1574-1	FMN, (scNH <sub>2</sub> ), scNH <sub>2</sub>	1569+0	FMN, scNH <sub>2</sub> , scNH <sub>2</sub>
1669 <sup>‡</sup>	1670-1	sC=O, sC=O	1651+0	sC <sub>2</sub> =O <sub>2</sub> , rN <sub>3</sub> -H, sC=O
1690 <sup>‡</sup>	1684-6	sC=O	1691-6	sC=O
		8.5 (7.0)		13.0 (14.5)
<b>1FMN*</b> <b>Excited State (<math>S_1</math>)</b>				
1375 <sup>‡</sup>	1374+11	<i>rN-H, rC-H</i>	1381+0	<i>rN-H, rN<sub>3</sub>-H</i>
1413 <sup>‡</sup>	1421+135 <i>scCH<sub>2</sub>, sC-N, rN-D(H)</i>	1430-0 <i>CH<sub>3</sub>, rN<sub>3</sub>-H, CH<sub>2</sub></i>	1415+146 <i>scCH<sub>2</sub>, sC-N, rN-D(H)</i>	
1498 <sup>‡</sup>	1510+1	FMN, C <sub>6,9</sub> -H, CH <sub>3</sub>	1431+0	scCH <sub>2</sub>
1574 <sup>‡</sup>	1572-2	scNH <sub>2</sub>	1493+0	<i>rN-H</i>
1622 <sup>‡</sup>	1612-1 <i>scNH<sub>2</sub>, scNH<sub>2</sub>, sC<sub>2</sub>=O<sub>2</sub>, sC<sub>4</sub>=O<sub>4</sub></i>	1629-3 <i>rN<sub>3</sub>-H, scNH<sub>2</sub>, sC<sub>4</sub>=O<sub>4</sub></i>	1611+0 <i>rN<sub>3</sub>-H, sC<sub>2</sub>=O<sub>2</sub>, scNH<sub>2</sub></i>	
			1643+0 <i>sC=O, scNH<sub>2</sub></i>	
		6.0 (9.8)		10.8 (13.4)
<b>3FMN*</b> <b>Excited State (<math>T_1</math>)</b>				
1438 <sup>‡</sup>	1438+0	rN <sub>3</sub> -H, scCH <sub>2</sub>	1446+0	<i>rN<sub>3</sub>-H, scCH<sub>2</sub></i>
1491 <sup>‡</sup>	1471+1	FMN, C <sub>6,9</sub> -H	1493+0	<i>rN-H</i>
1567 <sup>‡</sup>	1565+0	scNH <sub>2</sub> , FMN, rC <sub>6,9</sub> -H	1564+0	<i>rC<sub>6,9</sub>-H, scNH<sub>2</sub></i>
1622 <sup>‡</sup>	1638-1	rN <sub>3</sub> -H, sC=O, sC <sub>4</sub> =O <sub>4</sub>	1642+0	<i>sC=O, rN<sub>3</sub>-H, sC<sub>4</sub>=O<sub>4</sub></i>
		9.5 (10.0)		8.3 (8.3)
<b>3FMN*</b> <b>Excited State (<math>T_{1-H}</math>)</b>				
1438 <sup>‡</sup>	1417+136 <i>sC-N, rN-D(H)</i>	1451+20 <i>rN<sub>3</sub>-H, scCH<sub>2</sub></i>	1423-5 <i>rN<sub>3</sub>-H</i>	
1491 <sup>‡</sup>	1510+0 <i>rN-H</i>		1492+0 <i>rN-H</i>	
1567 <sup>‡</sup>	1587-10 <i>FMN (rN<sub>5</sub>-H)</i>		1523-1 <i>FMN, rN-H</i>	
1622 <sup>‡</sup>	1641+0 <i>rN<sub>3</sub>-H, sC<sub>2</sub>=O<sub>2</sub>, sC=O</i>		1584-8 <i>FMN (rN<sub>5</sub>-H)</i>	
		19.8 (18.8)		16.8 (14.5)
<b>A390</b> <b>Adduct State (<math>S_0^+</math>)</b>				
-	-	-	-	-
1418 <sup>‡</sup>	1410+3	CH <sub>2</sub> /CH <sub>3</sub> , rN <sub>5</sub> -H	1417+3	scCH <sub>2</sub>
1450 <sup>‡</sup>	1483+0 <i>rN-H</i>		1465+1	rN <sub>3</sub> -H
1555 <sup>†</sup>	1555+0	scNH <sub>2</sub> , FMN	1545-1	scNH <sub>2</sub> , FMN (rN <sub>5</sub> -H)
-	-	-	1561+1	scNH <sub>2</sub> , FMN
1639 <sup>†</sup>	1638+0 <i>sC=O</i>		1635-8 <i>sC=O, sC=O (sC=O)</i>	
1663 <sup>†</sup>	1659-12 <i>sC=O</i>		1644+0 <i>sC=O, scNH<sub>2</sub></i>	
1687 <sup>†</sup>	1691+0 <i>rN<sub>3</sub>-H, sC<sub>2</sub>=O<sub>2</sub></i>		1682#+0 <i>sC<sub>2</sub>=O<sub>2</sub>, rN<sub>3</sub>-H</i>	
-	-	-	-	-
1719 <sup>†</sup>	1703-4 <i>sC<sub>2</sub>=O<sub>2</sub>, sC=O, sC<sub>4</sub>=O<sub>4</sub></i>		1716+0 <i>sC=O</i>	
1713+0 <i>sC=O</i>			1726-1 <i>sC<sub>4</sub>=O<sub>4</sub>, rN<sub>3</sub>-H (rN<sub>5</sub>-H)</i>	
MAD	8.0 (9.0)		7.6 (7.7)	
		11.3 (11.3)		8.5 (8.1)

**Table S10** EL222 and AsLOV2 IR spectral assignments for the **Qb** and **Qd** models. Normal modes are coloured according to residue; FMN black, Q138/Q513 red, C75/C450 orange, N107/N482 green, N117/N492 violet, Q454 grey, A39/N414 blue, and light blue for backbone modes of other residues. Isotopic shifts from the non-deuterated spectra are given with red numbers. Mean absolute deviations are included for each theoretical/experimental correlation. All values are given in  $\text{cm}^{-1}$ .

### EL222

Exp.	Qb	Assignment	Qd	Assignment
<b>1FMN*</b>		<b>Ground State (<math>S_0</math>)</b>		
1547 <sup>†</sup>	1528+1	sFMN	1528+0	sFMN
1579 <sup>†</sup>	1573+0	sFMN, scNH <sub>2</sub>	1575+0	sFMN, scNH <sub>2</sub>
1655 <sup>†</sup>	1669+0	sC=O, sC <sub>2</sub> =O <sub>2</sub>	1669+0	sC=O, sC <sub>2</sub> =O <sub>2</sub>
1699 <sup>†</sup>	1689+0	sC=O, sC=O	1686-1	sC=O, sC=O
MAD	12.3 (12.5)		12.5 (12.3)	
<b>1FMN*</b>		<b>Excited State (<math>S_1</math>)</b>		
1378 <sup>‡</sup>	1403-13	scCH <sub>2</sub> , CH <sub>3</sub>	1402-2	CH <sub>3</sub>
1419 <sup>‡</sup>	1454+9	scCH <sub>2</sub> , CH <sub>3</sub>	1439+2	scCH <sub>2</sub> , rN <sub>3</sub> -H
1498 <sup>‡</sup>	1535+16	rN-H	1483+0	rC <sub>6,9</sub> -H
1571 <sup>†</sup>	1593-3	sC <sub>2</sub> =O <sub>2</sub> , rN <sub>3</sub> -H, scNH <sub>2</sub>	1570-11	rN-H
			1570*-1	scNH <sub>2</sub> , sFMN, rN-H
1623 <sup>†</sup>	1631#-10	rN <sub>3</sub> -H, sC=O, scNH <sub>2</sub>	1630-2	sC=O, rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , scNH <sub>2</sub>
1639 <sup>†</sup>	1643#-1	sC=O	1652+0	sC <sub>4</sub> =O <sub>4</sub> , sC=O
MAD	21.8 (22.2)		13.3 (16.7)	
<b>3FMN*</b>		<b>Excited State (<math>T_1</math>)</b>		
1428 <sup>‡</sup>	1448+0	rN <sub>3</sub> -H, scCH <sub>2</sub> , rC <sub>6,9</sub> -H	1447+0	scCH <sub>2</sub> , rN <sub>3</sub> -H
1488 <sup>‡</sup>	1469+0	sFMN, CH <sub>3</sub> , rC <sub>6,9</sub> -H	1470+0	sFMN, CH <sub>3</sub> , rC <sub>6,9</sub> -H
1567 <sup>†</sup>	1561+0	sFMN, scNH <sub>2</sub> , scNH <sub>2</sub> , CH <sub>3</sub> , rC <sub>6,9</sub> -H	1562+0	sFMN, scNH <sub>2</sub> , rC <sub>6,9</sub> -H
1639 <sup>†</sup>	1640+0	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , sC=O, sC <sub>4</sub> =O <sub>4</sub>	1638+0	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , sC=O, sC <sub>4</sub> =O <sub>4</sub>
MAD	11.3 (11.3)		10.5 (10.5)	
<b>3FMN*</b>		<b>Excited State (<math>T_{1-H}</math>)</b>		
1428 <sup>‡</sup>	1419+0	CH <sub>3</sub> , scCH <sub>2</sub>	1414+0	scCH <sub>2</sub> , CH <sub>3</sub>
	1418-131	sC-N	1417-129	sC-N
1488 <sup>‡</sup>	1508#+0	rN-H	1503#+0	rN-H
1567 <sup>†</sup>	1588-9	sFMN, scNH <sub>2</sub>	1553+7	rN-H
1639 <sup>†</sup>	1649+0	sC <sub>2</sub> =O <sub>2</sub> , rN <sub>3</sub> -H, sC=O	1650+0	rN <sub>3</sub> -H, sC <sub>4</sub> =O <sub>4</sub>
MAD	15.5 (17.5)		12.5 (15.0)	
<b>A390</b>		<b>Adduct State (<math>S_0</math>)</b>		
-	-	-	-	-
1418 <sup>‡</sup>	1409+2	CH <sub>3</sub> /rN <sub>5</sub> -H, scCH <sub>2</sub>	1409+3	(rN <sub>5</sub> -H), scCH <sub>2</sub> , CH <sub>3</sub>
1450 <sup>‡</sup>	1478+0	rN-H	1494+0	rN-H
1555 <sup>†</sup>	1558+0	scNH <sub>2</sub> , sFMN	1556+0	scNH <sub>2</sub> , sFMN
-	-	-	-	-
1639 <sup>†</sup>	1628-3	sC=O	1641#+0	sC=O
1663 <sup>†</sup>	1643+0	sC=O	1664-19	sC=N
1687 <sup>†</sup>	1687-1	rN <sub>3</sub> -H, sC=O, sC <sub>2</sub> =O <sub>2</sub>	1688-1	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub>
-	-	-	-	-
1719 <sup>†</sup>	1714+0	sC=O	1713+0	sC=O
	1726-1	sC <sub>4</sub> =O <sub>4</sub> , rN <sub>3</sub> -H	1724+0	sC <sub>4</sub> =O <sub>4</sub> , rN <sub>3</sub> -H
MAD	11.3 (11.3)		9.4 (12.7)	

FMN: ring breathing, *r*: rocking, *s*: stretch, *sc*: scissoring

#: Relatively intense ES peak in proximity to the experimental, offset by the GS signal

(): Normal mode only in non-deuterated spectrum

†: This study

‡: Taken from ref.<sup>32</sup>

### AsLOV2

Exp.	Qb	Assignment	Qd	Assignment
<b>1FMN*</b>		<b>Ground State (<math>S_0</math>)</b>		
1550 <sup>‡</sup>	1531+0	sFMN, rN <sub>3</sub> -H, scNH <sub>2</sub>	1533+0	sFMN, rN <sub>3</sub> -H
1583 <sup>‡</sup>	1577+1	sFMN, scNH <sub>2</sub>	1576+0	sFMN, scNH <sub>2</sub> , scNH <sub>2</sub>
1669 <sup>‡</sup>	1654+0	sC <sub>2</sub> =O <sub>2</sub> , rN <sub>3</sub> -H	1652+0	sC <sub>2</sub> =O <sub>2</sub> , rN <sub>3</sub> -H, sC=O
1690 <sup>‡</sup>	1692+0	sC=O	1691+0	sC=O
		10.5 (10.8)	10.5 (10.5)	
<b>1FMN*</b>		<b>Excited State (<math>S_1</math>)</b>		
1375 <sup>‡</sup>	1373+0	rN <sub>3</sub> -H	1365+0	sFMN, rN-H
	1380-97	scCH <sub>2</sub>		
1413 <sup>‡</sup>	1417+0	rN <sub>3</sub> -H, rN-H	1437+1	scCH <sub>2</sub>
	1410+126	scCH <sub>2</sub> , sc-N, rN-D(H)		
1498 <sup>‡</sup>	1503+0	sFMN, rC <sub>6,9</sub> -H	1489#+0	sFMN, CH <sub>3</sub>
1574 <sup>‡</sup>	1587+0	scNH <sub>2</sub> , rN <sub>3</sub> -H, sC <sub>4</sub> =O <sub>4</sub>	1562-1	scNH <sub>2</sub> , rN-H, rN-H
1622 <sup>‡</sup>	1615+0	scNH <sub>2</sub> , rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub> , scNH <sub>2</sub>	1629+0	sC <sub>2</sub> =O <sub>2</sub> , rN <sub>3</sub> -H, scNH <sub>2</sub> , scNH <sub>2</sub>
	-	-	-	-
		6.6 (6.2)	12.4 (12.0)	
<b>3FMN*</b>		<b>Excited State (<math>T_1</math>)</b>		
1438 <sup>‡</sup>	1444+0	rN <sub>3</sub> -H, scCH <sub>2</sub>	1447+0	rN <sub>3</sub> -H, scCH <sub>2</sub>
1491 <sup>‡</sup>	1485+0	rN <sub>3</sub> -H, sFMN	1485+0	rN <sub>3</sub> -H, sFMN
1567 <sup>‡</sup>	1562+0	scNH <sub>2</sub> , C <sub>6,9</sub> -H	1564+1	sFMN, rC <sub>6,9</sub> -H, scNH <sub>2</sub>
1622 <sup>‡</sup>	1640+0	rN <sub>3</sub> -H, sC=O, sC <sub>4</sub> =O <sub>4</sub>	1641+0	sC <sub>4</sub> =O <sub>4</sub> , rN <sub>3</sub> -H, sC=O
		8.8 (8.8)	9.3 (9.5)	
<b>3FMN*</b>		<b>Excited State (<math>T_{1-H}</math>)</b>		
1438 <sup>‡</sup>	1419-3	rN <sub>3</sub> -H/CH <sub>2</sub> , rN <sub>3</sub> -H	1410+146	sC-N, rN-D(H)
			1417-4	rN <sub>3</sub> -H
1491 <sup>‡</sup>	1488+0	rN-H	1494-1	rN-H
			1525+0	sFMN, rN-H
1567 <sup>‡</sup>	1587-9	rN <sub>5</sub> -H, scH <sub>2</sub> O, sFMN	1584#-8	rN <sub>5</sub> -H, sFMN
1622 <sup>‡</sup>	1644+0	sC=O, scNH <sub>2</sub> , rN <sub>3</sub> -H, sC <sub>4</sub> =O <sub>4</sub>	1643+0	sC=O, scNH <sub>2</sub> , rN <sub>3</sub> -H, sC <sub>4</sub> =O <sub>4</sub>
		16.0 (17.5)	17.3 (16.8)	
<b>A390</b>		<b>Adduct State (<math>S_0</math>)</b>		
1389 <sup>‡</sup>	1373-8	sC-N/rHNCOH	1372+5	FMN, scCH <sub>2</sub>
1417 <sup>‡</sup>	1408#+0	rN-H, scCH <sub>2</sub>	1407#+0	rN-H, scCH <sub>2</sub>
1435 <sup>‡</sup>	1456-2	rN <sub>3</sub> -H	1429+8	CH <sub>3</sub> , rN <sub>5</sub> -H/CH <sub>3</sub> , CH <sub>2</sub>
1541 <sup>‡</sup>	1548+0	scNH <sub>2</sub> , FMN	1548-1	scNH <sub>2</sub> , FMN
	1561+0	scNH <sub>2</sub>	1561+0	scNH <sub>2</sub>
1610 <sup>‡</sup>	1620-2	sFMN	1621-1	sFMN
1634 <sup>‡</sup>	1640+0	sC=O	1641+0	sC=O, scNH <sub>2</sub>
1665 <sup>‡</sup>	1666-1	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub>	1667-1	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub>
1671 <sup>‡</sup>	1682#-5	sC=O	1679#+0	sC=O, sC <sub>2</sub> =O <sub>2</sub>
1695 <sup>‡</sup>	1704+0	sC=O (side ch.)	1682-5	sC=O
1722 <sup>‡</sup>	1727-1	rN <sub>3</sub> -H, sC <sub>4</sub> =O <sub>4</sub>	1704+0	sC=O (side ch.)
		9.5 (9.8)	1727-1	rN <sub>3</sub> -H, sC <sub>2</sub> =O <sub>2</sub>
			8.6 (9.8)	

### 3. Cartesian coordinates of all optimised ground-state and excited-state species

EL22 Qa	S	C	15.46499756	-9.61300565	29.59100173	C	1.56094945	-8.98809246	18.23480108	N	6.55322072	-7.14533942	19.07016050
		C	14.06103527	-9.05222260	29.74087843	H	7.15014848	-6.32649605	19.16365247	C	5.63445344	-3.74650284	18.03799282
O		C	13.31016706	-9.35450693	30.66707599	H	4.68510694	-10.64377652	23.92332288	O	5.74045119	-7.62705896	16.99513583
H		C	16.07699962	-8.80499893	29.19000312	H	1.79473483	-1.31741906	25.09125296	N	4.63909057	-8.31204195	18.20570257
H		C	15.81200321	-9.88599579	30.58800236	H	2.91593605	-13.59745918	25.45798586	C	4.53281378	-9.82949844	19.35988533
H		C	15.48128405	-10.48194612	28.91696852	H	3.54158395	-12.1527625	25.39144018	C	5.43080635	-8.72212892	18.49550640
N		C	13.70631301	-8.11759630	28.01844012	H	0.38724046	-13.23303513	25.50190678	N	5.31865544	-9.32061951	21.63930493
C		C	12.31901008	-7.66550513	28.76126249	H	1.32552249	-14.04559490	22.79062137	C	4.27148684	-10.18179912	18.20922607
C		C	11.43801547	-8.87870850	28.45700701	H	0.23767957	-12.70926015	23.20486190	C	4.11657214	-9.70996349	23.07069081
O		C	11.68880273	-9.59541865	27.48416634	H	1.50934473	-11.65359308	20.28366557	C	3.07593444	-11.67194770	23.33903644
C		C	12.14085975	-6.59058693	27.68952124	H	2.16270142	-11.10480445	18.51856524	C	2.92173705	-12.30629861	24.96811783
H		C	14.18162282	-8.14442529	27.90052585	H	3.27153301	-10.11139907	17.56194544	C	2.14563068	-11.95674151	22.29379214
H		C	12.06805655	-7.26718825	27.95634777	H	2.14197889	-8.07300111	18.34611627	C	0.99361668	-12.89386395	25.57241743
H		C	11.07497157	-6.35491017	27.55886758	H	1.14185391	-0.46663232	7.21921027	C	2.28057550	-11.34892402	21.04379425
H		C	12.68960156	-5.76836888	27.97053330	H	0.74306622	-8.98692620	18.95507635	C	3.33805295	-10.45480400	26.79069283
H		C	12.53086492	-6.95805030	26.79298647	O	0.03329284	-9.94078661	23.22802523	O	3.51624131	-9.84533537	19.53877114
H		C	10.40424613	-9.11266813	29.28942383	H	0.72099654	-10.09703180	23.89499503	C	2.60208213	-10.10152319	18.39628783
C		C	9.57603150	-10.29200942	29.12699171	H	0.45440004	-10.25352457	24.41024368	C	1.56130718	-18.89719518	18.24350786
H		C	10.40049558	-8.63210539	30.18128858	H	0.27553295	-6.42150358	18.88857292	H	7.27553295	-6.42150358	18.88857292
H		C	9.58390197	-10.54799533	28.06700062	C	15.46501185	-9.61300888	25.99101321	H	4.85900959	-10.54473734	23.82916167
H		C	9.94589710	-11.17399660	29.07801256	C	14.05061880	-9.08687307	29.74069777	H	1.93802259	-12.07519911	25.13818267
H		C	8.54468892	-10.07159563	29.43957528	H	0.23769726	-8.80499723	23.19986642	H	2.99115325	-15.40531794	24.63655180
C		C	-2.49301852	-7.05709373	23.10698713	H	16.07697266	-8.80499723	23.19986642	H	3.69912453	-11.95442278	25.38876265
C		C	-1.19322721	-6.32685504	22.90066230	H	15.81189649	-8.98598718	30.58801014	H	0.40551377	-13.07038219	26.15399181
O		C	-1.16949844	-5.10201723	22.69946736	H	15.49408717	-10.48647106	28.92254466	C	1.34983065	-13.86626449	22.92364198
O		C	-2.34441762	-8.04129519	23.57918808	H	13.69893792	-8.10456674	28.85309681	H	0.3173970	-12.47691615	23.11124473
H		C	-3.09800662	-6.43603073	23.76702441	C	12.31789013	-7.64076437	23.84834776	H	1.55293269	-11.58977294	22.07267929
H		C	-3.02497673	-7.22605012	22.69969695	H	11.42358428	-8.83360416	28.47872809	H	2.17621941	-11.10321286	18.51573803
N		C	-0.07543858	-7.08587233	22.94639316	H	11.65916246	-9.5158879	27.04803600	C	3.24286254	-10.11415973	17.50631888
C		C	1.25910271	-5.26187603	22.72903906	C	12.16816122	-6.50808910	27.81942907	H	2.14170559	-8.07229274	18.34689876
C		C	1.51953334	-6.36354322	21.21022029	H	14.19832133	-8.05195144	27.96735544	H	1.13635263	-9.03484426	22.17231781
O		C	2.45034321	-6.93441961	20.62980492	H	12.06920704	-7.28877674	29.84753416	H	0.74296055	-8.98716258	18.59455957
C		C	2.30529660	-7.40829352	23.41832937	H	11.12154343	-6.17673534	27.75040559	O	-0.35658378	-9.91772205	22.27912380
S		C	3.95942207	-6.62329067	23.58313489	H	12.79850092	-5.65726193	23.18021717	H	0.53292555	-10.22422524	21.97787719
H		C	-0.15355056	-8.10431300	23.03306557	H	12.48869092	-6.85445190	26.82575009	H	0.87429540	-10.03421290	21.41565383
H		C	1.26841329	-5.52238226	23.17804754	N	10.37057896	-8.08496883	27.04939616	H	9.15158949	-7.91746374	27.06770301
H		C	1.97894981	-7.61563903	24.44154945	C	9.57600135	-29.22988998	29.12696054	C	15.46501111	-9.61300369	29.59101331
H		C	2.41468810	-8.36383872	22.88114860	H	10.38711714	-8.65131284	20.31065093	C	14.05308699	-9.08052385	29.75070245
H		C	4.42219647	-5.69431217	22.55928483	H	9.58399843	-10.54799909	28.06700131	O	13.29382579	-9.44120226	30.64899411
N		C	1.51093030	-5.55330730	20.62475579	H	9.94596297	-11.13801283	29.70800959	H	16.07697014	-8.80498661	29.18995809
C		C	0.69799297	-5.07050928	19.26898620	C	-2.49259357	-7.05748307	23.10670905	H	15.81199611	-9.88599470	30.58800522
H		C	-0.06428191	-5.10572023	21.25232603	H	1.17692053	-6.34960657	22.19893252	C	15.48914699	-10.48563285	28.92149281
H		C	1.59024400	-5.48295777	18.81201122	O	-1.11508485	-5.11545684	22.80300862	N	13.69448748	-8.10470920	28.81851563
H		C	-0.16301524	-5.28496126	18.63400906	H	-2.35690007	-8.04352193	23.57387447	C	12.31463833	-7.63563819	28.88518463
H		C	0.81144457	-3.77955903	19.27522155	H	-3.09807850	-6.43632441	23.76723539	C	11.41299481	-8.81826572	24.87791745
C		C	8.88899299	-1.76498056	16.94499816	H	-3.02520825	-7.22188724	22.17010051	O	11.63920951	-9.46713561	24.45567760
C		C	8.76371283	-6.53652786	18.68529574	H	-0.08425038	-7.14770204	22.90008444	C	12.16530318	-6.48833570	28.75854543
C		C	8.08837090	-4.01319396	18.04262200	H	1.25911419	-6.61300462	22.69307972	C	14.18689482	-8.06413268	27.96554453
O		C	8.17683473	-8.43706477	18.97996851	H	1.51903303	-6.39943287	21.18285087	H	12.07444124	-7.29493153	29.87104477
N		C	7.37293988	-4.28800456	16.94550469	C	0.244833010	-6.95104734	20.58411338	H	11.23551557	-6.33535553	27.83672482
H		C	7.93503746	-1.71071879	18.36920418	C	2.29064988	-7.35539253	23.33862415	H	12.81825690	-6.535263509	28.14435472
H		C	9.74749192	-2.87148324	18.64247188	S	3.94308001	-6.76492884	23.57278810	C	12.44651961	-6.82889407	24.86712318
H		C	8.17590301	-2.13868294	18.96707428	H	-0.21622817	-8.15706832	22.76736557	N	10.38465424	-9.07122620	23.09384344
H		C	7.26162083	-3.60945045	16.20395960	H	1.28657740	-5.62516878	23.17816766	C	1.51686912	-6.88719720	23.02636444
H		C	6.83338737	-5.61650150	16.19796207	H	1.94867858	-7.80512247	24.43805574	H	10.42277878	-8.68719720	23.17800811
H		C	9.10001842	-7.31017301	17.21899392	H	2.40922987	-8.45723521	22.75258829	H	9.94597577	-11.13801579	29.70800811
C		C	13.2199376	-5.73700863	18.45901888	H	0.60715057	-5.57394762	20.61825060	N	8.08167587	-10.08086410	24.44364436
C		C	11.77435752	-5.77123555	18.92348913	H	0.69863062	-5.07631404	19.26189429	C	1.25857876	-6.88856219	23.98811393
H		C	11.97900158	-12.35993959	25.69502028	H	9.10032132	-7.03965282	17.21826529	H	2.14091807	-6.43407957	22.77349249
H		C	9.94871011	-12.23922555	23.04423466	H	9.65281279	-6.12330135	23.15395620	H	4.23657851	-6.67105823	22.23892308
H		C	11.69194033	-5.53690303	24.65395035	C	13.21281612	-5.73028252	18.45919901	N	0.60539581	-5.56961000	16.29117281
C		C	12.13658480	-8.50396548	23.74494449	H	11.77887563	-5.52935662	19.95144836	C	2.44414468	-6.95009969	20.58996217
C		C	13.60167313	-8.16887879	24.05272128	H	11.43336702	-6.43426559	20.14292539	C	2.29826178	-7.50488112	23.35118349
C		C	14.01641638	-8.07616278	25.21492962	O	12.26579495	-7.18369413	26.67168872	H	0.05194373	-11.51681667	21.25835958
C		C	11.26775502	-7.23503025	23.85509459	N	10.15465941	-6.32784873	20.56566353	H	-0.16359001	-5.28352328	18.63434553
C		C	9.79551190	-7.49655425	23.51798888	H	13.87517268	-5.50829709	19.29448447	H	0.81260929	-9.37711755	23.18292214
C		C	8.91835377	-7.93026126	20.75091064	H	11.61161064	-4.48338749	21.25938710	H	8.88991065	-7.16458132	23.94577211
O		C	9.26270111	-7.83434234	25.88399498	H	11.03548394	-7.50259527	18.1509984	C	8.74943600	-2.66980483	18.12981385
N		C	7.69594469	-8.40741615	20.37337993	H	9.48459637	-5.76394089	20.04199314	H	8.11914202	-4.05423248	17.97307134
H		C	11.77269812	-9.35302171	25.65700133	H	9.77744229	-7.00722707	21.21747270	O	0.34612473	-4.95495713	18.79938979
H		C	12.04760946	-8.89909749	22.73292020	H	13.32594913	-6.78002513	18.216406903	N	7.2858146	-4.23939934	16.94093870
H		C	11.34624206	-10.81904404	24.86959865	H	13.447425						

C	9.12526906	-8.29229332	25.17702153	H	9.76207943	-7.02015011	21.19030232	H	9.73481389	-2.87235949	18.63317000
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H	11.36124329	-6.78644951	24.80926668	O	11.14543702	-11.08363404	23.06753903	H	9.65299875	-2.12300131	16.25399925
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H	16.07697014	-8.08499681	29.18959809	H	0.26109930	-12.49254558	23.26950741	C	2.88024488	-11.88403151	23.29425555
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N	11.80041712	-5.78815175	24.66618168	H	12.44358555	-7.02486062	20.65206577	C	8.88981710	-1.76457324	16.94532655
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C	9.15239871	-8.28366456	25.18381728	H	9.76811649	-7.02065267	21.21067067	H	9.71831924	-2.87414732	18.64082069
O	9.47259852	-7.48278947	26.24830473	H	13.32594215	-6.78002463	18.16406278	H	8.14362668	-2.15297244	18.95058300
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H	12.03750646	-8.88848368	22.72812686	C	11.23942107	-10.75320497	24.24929938	H	9.05970415	-4.01915831	17.99142463
H	11.38544346	-7.87523286	20.87302302	H	11.07512768	-5.01452222	23.06519218	H	9.65283640	-2.12331444	16.25398263
C	11.36648934	-6.60545774	23.08470274	H	10.50803361	-11.02005673	26.24405427	C	13.21283168	-5.73699910	18.45916885
H	9.07388077	-6.81981815	23.66947355	H	11.57897766	-12.34606040	25.692942016	H	11.77675178	-5.52677476	18.94219353
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O	5.56487865	-6.63269041	17.097187912	H	11.37156732	-6.76651677	18.247611071	O	11.15778511	-11.09452520	23.06743875
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C	5.44548208	-22.92632366	22.462699302	H	9.49894678	-8.33801574	23.12299030	C	11.74021003	-9.55332020	24.65224046
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H	3.25479443	-10.09356595	17.51280074	C	0.82066894	-13.03984220	22.41152937	O	7.39193575	-7.53338843	21.17961940
H	2.14170695	-8.07292972	18.34695253	C	2.14272954	-11.38370824	21.04882080	C	6.54126787	-7.79383328	20.33028557
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H	-0.89130205	-10.04588661	21.38554782	H	7.14161524	-6.32146664	19.21964450	C	4.56430444	-8.94993740	19.41599175
H	8.15017076	-9.63423804	25.76320609	H	4.72693210	-10.86580082	23.90337460	C	5.45427780	-8.76454079	20.50723149
El222 Qa T <sub>i</sub>				H	1.80424979	-12.48781169	25.04192305	N	5.36424083	-9.42274775	21.69499359
C	15.46499703	-9.61300554	29.59100263	C	2.84550918	-13.75746598	24.39903186	C	4.2978459	-10.23778559	21.82272179
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O	13.31029813	-9.35507042	30.66729058	H	0.21039604	-13.09850589	21.49964421	C	3.03176022	-11.74768686	23.30189475
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H	15.81200337	-8.88599792	30.58800204	H	0.16512204	-12.71261164	23.23559911	C	2.07343124	-11.99242606	22.25762955
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H	14.18168643	-8.14269280	27.90172539	H	0.06762663	-9.29721311	23.40973928	H	7.25988978	-6.41154774	18.94598668
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H	9.10001985	-7.03100209	17.21893494	C	0.69683105	-5.07631430	19.26814939	H	-2.35754025	-8.04376920	23.57812284
H	9.65303019	-12.23030090	16.25400814	H	-0.04222001	-5.11643181	21.26294624	H	-3.09807922	-6.43652245	23.76723269
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C	0.86046141	-12.91962737	22.46919482	O	7.37087894	-7.57841521	21.24011023	N	7.61102037	-7.95985333	24.36619498
C	2.21010516	-11.36267958	21.25259028	C	6.52176409	-7.82157397	20.3897463	C	12.04755444	-8.90541740	22.71837000
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C	2.60213908	-10.10738128	18.39388244	O	5.67846633	-6.69125304	17.09350085	H	9.40131115	-6.54729637	23.04038287
C	1.56126911	-8.97813655	18.23446532	H	4.64716177	-8.33365074	22.81982478	H	9.68960167	-8.26561647	22.80130472
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H	1.48482017	-11.55176625	20.23217071	C	0.83985011	-12.93051769	22.45030543	H	15.82100372	-6.87535610	22.27210704
H	2.17022986	-11.10605003	18.48981911	C	2.0009848	-11.37622392	21.01046272	O	7.16276507	-7.48021384	21.45481183
H	3.25078826	-10.10644242	17.51500583	C	3.29060111	-9.51210695	20.77018940	C	6.38433809	-7.72601404	20.51410153
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O	-0.37932594	-9.90672881	22.23939191	H	-0.38528812	-9.40807944	19.02326465	N	4.62697943	-8.29040416	18.31878347
H	0.50462235	-10.23294521	21.98245637	H	4.78093188	-10.75684524	23.84365120	C	4.48755010	-8.93110324	19.46658273
H	0.89701301	-10.01369949	21.41591106	H	1.81007633	-12.23894038	25.04598149	C	5.33803078	-8.72249072	20.58428435
H	1.72222222	-7.66088026	28.06818593	H	2.83288857	-13.57260378	24.50627968	N	5.71080480	-9.43356090	21.73126125
H	12.54166723	-8.69974061	28.78565972	C	3.57369903	-12.17245444	25.32746821	C	4.11676651	-10.30130745	21.90113363
N	10.38801065	-9.09948118	29.29453753	C	0.25058084	-10.05481604	21.52781834	C	3.91227988	-10.95952489	23.12365193
C	9.57603971	-10.29929672	29.12698912	H	1.15247074	-13.92954135	23.794737816	C	2.85891089	-11.85220431	23.30646336
H	10.40498841	-8.65349564	30.20459244	H	0.16695671	-12.51650486	23.21939263	C	2.67000400	-12.55959459	24.62377180
H	9.58401568	-10.54799753	28.06700099	H	1.47321331	-11.55676163	20.21946919	C	1.97045883	-12.08351012	22.22414838
H	9.94595873	-11.13806981	22.89955986	H	2.16413106	-10.11834636	18.478424415	C	0.81816361	-13.04610518	22.37545271
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C	1.51191741	-6.41225909	21.17234533	H	12.53151400	-9.63662882	26.72266414	H	1.24198216	-8.07300592	18.34611531
O	2.42714889	-6.97490709	20.56243076	N	10.40483441	-9.11233846	29.28910331	H	1.13494985	-9.03470456	17.22080820
C	2.30016862	-7.54991503	23.31754549	C	9.57603235	-10.29301604	26.12699541	H	1.17262447	-14.04852596	22.66569538
S	3.95741149	-7.63084947	23.52151478	H	10.40996966	-8.636901121	18.49252959	C	0.00657494	-9.92185746	23.30190063
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N	0.59189056	-5.59236374	20.61100410	C	-1.16408369	-6.36649275	22.92954490	C	11.42390189	-8.85346569	28.45546334
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H	0.81300925	-3.97771202	19.29719849	N	-0.07985890	-7.17968816	22.89080764	H	11.10197882	-6.28319072	27.61642054
C	8.88998707	-1.76466087	16.94542452	C	1.26715110	-6.65900701	22.67406601	H	12.73799855	-5.66478673	28.03963237
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H	9.10031301	-0.73096277	19.21862392	C	0.69863605	-5.07632639	19.26819937	O	-1.10476561	-5.12013846	22.81653338
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<b>El222 QaS</b>											
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C	12.43934843	-8.56214011	27.5392196	H	0.74288305	-8.98718566	18.95486839	C	1.56108911	-8.98771166	18.23554331
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H	0.74279536	-8.98726556	18.95476872	C	1.56050311	-8.98783766	18.23458332	C	14.07320064	-2.94090777	4.19642450
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O	13.29050759	-9.41815257	30.64048082	H	0.26164010	-12.98548711	23.72220327	H	15.86843002	-3.99256199	3.78072739
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C	12.31641325	-6.56628476	28.70044285	H	1.17063373	-9.08025608	25.12623888	H	14.99249165	-4.41750019	1.26888018
C	11.42423210	-8.85400794	28.45989737	H	0.74317905	-8.98795564	18.95252035	H	13.08999955	-6.62896546	1.81294813
O	-1.035554812	-5.14733655	23.08939532	C	0.22161596	-10.05544096	23.02802865	C	12.05621453	-0.88544165	4.82105217
H	-2.37839326	-8.05126848	23.57482930	C	17.77357284	-0.08583211	9.64488112	C	19.94850309	-1.41159274	4.84627074
H	-3.09822022	-6.43952394	23.76734649	S	16.11350581	-0.25518194	10.35742241	C	18.52368471	-1.16192544	5.09200941
H	-3.02518222	-7.22171351	22.17003658	H	18.43955923	-1.95182994	11.35078111	O	17.63194643	-1.94798651	4.78174879
N	-0.06231515	-7.17759907	22.77326774	H	18.90571719	-9.69168688	11.17538808	C	18.75563306	-3.83183337	7.49306878
C	1.26850580	-6.58660117	22.66124240	H	1.719766330	-6.05733082	8.85087309	C	17.87875788	-2.59337288	6.89887500
C	1.27590618	-5.46157652	21.61060347	H							

H	21.18120889	-0.03876603	11.71813095	H	14.85869415	0.94370308	6.95754685	H	13.79216964	-5.26984164	2.53260847								
H	22.71792776	0.02805125	9.14600059	H	13.76374403	3.38249762	9.26026488	H	15.08952868	-2.50433087	2.92248508								
H	23.15844660	-0.93487926	10.55351385	H	13.35714069	4.04944574	7.67286167	H	15.52980897	-3.85160693	3.99100788								
H	23.37795001	0.80609787	10.60788719	H	13.16636351	2.30308422	7.97463833	H	12.20527841	-4.112677673	5.45968800								
C	25.51302633	-3.72099198	7.23808824	H	16.70756167	5.94785666	8.55889797	H	13.52426963	-5.11263750	4.92088152								
C	25.86549891	-2.22856057	7.26617715	H	15.04200565	5.575793780	7.94929857	N	14.13481778	-4.95471639	-1.22330032								
C	24.69982340	-1.36742054	6.77920523	H	15.47389945	5.11688529	9.54208198	C	13.90699099	-6.01799608	-2.19603123								
C	24.74711497	0.08374613	7.25699042	H	18.27064813	4.48779989	7.66389682	H	14.99164682	-4.40963350	-1.28245734								
O	25.43069915	0.04473524	8.21544949	H	19.85453760	4.18720149	6.42490513	H	13.09000895	-6.62900747	-1.81299451								
N	23.94287345	0.92806696	6.56262404	H	21.06082847	2.97473075	5.96490955	H	13.66781436	-5.61779664	-3.19207903								
H	25.32086043	-4.08038536	6.21189536	H	21.49783003	2.34288383	8.25094664	H	14.81299996	-6.62020070	-2.23099316								
H	26.76606365	-2.01992772	6.66299243	H	21.45109416	4.12482615	8.26206603	O	16.32074236	2.68720171	11.56193656								
H	26.10940327	-1.92702944	8.29754604	H	20.05584748	3.19802359	8.86188786	H	15.88893103	2.97735646	12.38050905								
H	23.74562485	-1.71583393	7.16804160	H	12.20514315	-4.14124813	5.20396535	H	15.98878974	1.77335189	11.43001638								
H	24.59924337	-1.39558052	5.68307726	<b>AsLOV2 Qe So</b>															
H	23.81340288	1.86369894	6.93025406	C	19.02907417	-1.11990453	13.81299636	C	21.00508060	-0.45461221	4.90283485								
H	23.2782079	0.56749488	5.87742401	C	19.33683297	0.94137451	9.12018151	O	22.16928431	-0.77184146	4.59539024								
H	26.30801185	-4.33201336	7.66594628	O	20.08916876	0.01870353	13.25594555	N	19.97747871	-1.35091718	4.60810285								
H	24.60697518	-0.83409961	7.83195992	H	18.15299028	2.65196183	13.45296935	C	18.65315581	-1.19719615	4.95276266								
C	23.25601503	-6.51499555	3.78394899	H	18.86871029	1.74993126	14.83780584	O	17.79629317	-2.02046646	4.66095403								
C	21.82557400	-5.95419197	3.94175514	H	19.8929381	2.77602368	13.81023620	C	18.38240973	0.06085473	5.71070825								
C	21.70614975	-4.42997373	3.98375749	N	18.77256492	1.00226515	11.68094281	N	17.17147703	0.26033455	6.15216871								
O	20.75055719	-3.84335483	3.43578834	C	18.93053094	-0.06186313	10.69669063	C	16.92712197	1.41232428	6.88323220								
N	22.63247336	-3.72132153	4.66528724	C	20.26933933	0.06556522	9.91551797	C	15.64945160	1.59245590	7.41974418								
H	23.91599922	-4.9273980	7.37425887	O	20.29728158	0.10289758	8.68303299	C	15.34613281	2.70271530	8.18634749								
H	23.379201435	-6.30535605	4.89659556	C	17.76925856	-0.03893478	9.71026811	C	14.01721120	2.83347969	8.88138561								
H	21.14920832	-3.60127033	3.14794073	S	16.10027966	-0.63732301	10.44908279	C	16.34061263	3.71958599	8.33205152								
H	22.55879797	-2.70899627	4.71708607	H	18.11922724	1.76186249	11.48518649	O	16.04577943	4.94480587	9.15173364								
H	23.35607462	-4.19231402	5.20155324	H	18.98202592	-0.10416247	11.25236766	C	17.59606054	3.56504671	7.75136210								
H	23.34100455	-7.52799273	4.17701805	H	17.95890558	-0.84472596	9.84005005	C	17.93264288	2.40332615	7.02841824								
H	23.58511994	-6.49723980	7.37425887	H	17.68954997	0.87975844	9.20141502	N	19.20347771	2.17265623	6.52085439								
C	19.24992407	-5.26294371	-0.04997246	H	16.46391852	-1.31497107	11.35261256	C	19.49690866	0.98001893	5.90236292								
C	19.36965688	-4.7812181	0.39467402	N	21.35275423	0.11553886	7.70224067	C	20.26343429	3.19558613	6.69966994								
C	18.07203606	-4.04169847	0.90956475	C	22.71300477	0.02611273	10.23604391	C	20.85330071	3.21119743	8.11817708								
O	17.06484051	-4.02246403	0.19893738	H	21.18148411	-0.03945809	11.71887238	H	20.23211658	-2.23394223	4.12723364								
N	18.12568473	-6.41301663	2.0086183	H	22.71798195	-0.02790578	9.14600059	H	14.92308629	0.79310189	7.26343464								
H	18.37503676	-5.91104672	-0.109600850	H	23.15908225	-0.93470128	5.55229008	H	14.17119236	2.91052179	9.97012673								
H	20.18289828	-0.04728089	0.52675662	H	23.37803500	0.08597672	10.60798672	H	13.47795122	3.74124968	8.56451020								
H	19.62117409	-5.61840884	1.06974080	C	25.51301088	-3.72099440	7.23809350	H	13.37523474	1.96493783	8.68016797								
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H	20.14328354	-5.82731489	-1.35760501	C	24.68746918	0.06658809	7.10955201	H	15.91108562	4.64683499	10.20360201								
H	19.12102597	-4.41301003	-1.72040162	O	25.30463717	4.42685675	8.10034708	H	18.32755485	4.35614451	7.89755147								
C	6.29800456	-6.61101053	1.89501106	H	23.15908225	-0.93470128	5.55229008	H	19.81507627	4.16306921	6.43472491								
C	7.35982067	-6.33631890	2.95003271	H	25.30277452	-0.14071327	6.22392700	H	21.03628200	2.96740315	5.95935642								
O	7.09241725	-6.15656784	4.13847731	H	26.74582088	-0.20409304	6.19618670	H	21.49782997	2.34264549	8.25094908								
H	6.67376179	-7.25558033	1.08635033	H	26.06583142	-0.88098624	8.24368935	H	21.44800206	4.12850994	8.24904340								
H	6.01600717	-5.65100055	1.46299620	H	23.71659848	-1.80726423	8.70151887	H	20.05581414	3.19797772	8.68158124								
H	5.42299405	-7.06889311	2.35499689	H	24.57386334	-1.48464321	8.59573809	<b>AsLOV2 Qd So</b>											
N	8.64271773	-6.26019236	4.28696608	C	23.78036597	1.82897373	6.66118796	C	19.0290836	2.11203215	13.81284798								
C	9.75810060	-6.01391040	3.39366577	H	23.30298862	-0.94814486	5.63020023	C	19.34352002	0.94059336	12.90990014								
C	9.93049215	-4.50102949	3.61224235	H	26.30802185	-0.43320100	7.66594913	O	20.11414238	0.03321346	12.35402214								
O	10.38029483	-3.77181623	2.72355451	H	24.60697619	-3.84099487	7.81926394	H	18.15296731	2.65196019	13.45302295								
C	11.07562944	-6.55115419	2.82684219	C	25.26603054	-6.51500663	3.78402139	H	18.86704105	1.74978466	14.83723988								
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H	8.83598654	-6.35221052	1.45989823	H	22.72850258	-6.33734894	4.14137516	C	20.26906109	0.06625919	9.91190311								
H	9.51071426	-6.51235963	4.33987177	H	23.91599109	-5.85789717	4.34996650	O	20.30452120	0.09817648	8.67862230								
H	11.82819813	-6.53186582	3.62953019	H	21.38716927	-6.22436346	4.87949097	C	17.55971876	-0.03126516	9.69995908								
H	11.42300907	-5.88095235	0.32204409	H	21.15803351	-6.35194847	3.12907724	S	16.10936849	-0.40214725	10.42870948								
H	11.28045136	-6.20291460	4.74082596	H	22.59281596	-6.16919810	4.20460557	C	18.10173793	1.74033077	11.17644523								
H	11.66102040	-4.08397980	1.57601325	H	23.62775935	-0.41885232	7.16122122	H	22.71796962	0.0279300	9.14600064								
C	12.85577176	-6.48514550	1.03138808	H	18.37498648	-5.61908192	10.05979891	H	23.15782995	-0.93520056	10.53324789								
O	13.79738807	-1.05327244	0.45090073	H	20.15940356	-4.03038633	5.52702067	H	23.37799970	0.80604306	10.6701275								
H	11.17399296	-4.15700338	2.33199200	H	19.57667679	-5.59011498	1.08686114	C	25.51300183	-3.72099727	7.23805154								
H	10.95099413	-5.07901418	0.79100187	H	17.29978827	-3.15893515	2.53379301	C	25.84662480	-2.22616827	7.22725945								
H	12.02650296	0.09306031	2.02805337	H	18.87645310	-3.86123332	2.74164026	C	24.67081184	-1.39794154	6.70339609								
N	12.80346005	-2.9																	

C	11.07890452	-6.51719184	2.80514216	C	23.25606859	-6.51493390	3.78395429	H	18.86571192	1.74908491	14.83648035
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O	10.57405726	-8.86864858	3.08915640	C	20.44908591	-4.03673269	3.80457517	N	18.77486689	0.99402037	11.67486473
N	11.49037550	-8.18044928	1.11517015	O	22.61848753	-3.64734774	4.24300616	C	18.93092301	-0.05431545	10.66719764
H	8.82866622	-6.32723938	1.49157764	N	23.91596410	-5.85800215	4.35004673	C	20.27983540	0.04051076	9.90577354
H	9.53040600	-6.50811194	4.33153555	H	21.38568096	-6.34027995	4.88326457	O	20.33028324	0.00307057	8.67714282
H	11.85636004	-6.40947305	3.57860363	H	21.15464535	-6.37186559	3.14395021	C	17.77522429	-0.00484586	9.67038291
H	11.37788506	-5.87479146	1.96890790	H	22.42853565	-2.63827237	4.39130323	S	16.12763003	-0.39809007	10.42194716
H	11.55107779	-9.13154971	0.76928342	H	23.54931650	-3.99005224	4.42159755	H	18.20314125	1.80606169	11.41309959
H	11.88235873	-7.41068122	0.57350633	H	23.34092401	-7.52801823	4.17697326	H	18.93859084	-1.02146202	11.19918217
N	9.59543151	-4.01883120	4.82894058	H	23.59263632	-6.50305576	2.75380173	H	17.94369972	-0.73341038	8.86938710
C	9.75200077	-2.59900510	5.11996370	C	19.24993662	-5.26289940	-1.04995596	H	17.72156403	0.98390788	9.19846447
H	9.01717694	-4.60469238	5.42306147	C	19.38860095	-4.75564097	0.38336303	N	21.35549352	0.14060138	10.72241458
H	10.66400077	-2.28999817	4.60900033	C	18.17015838	-3.94677983	0.84975881	C	22.71296292	0.02623452	10.23607471
H	9.84858202	-2.45218021	6.20456313	O	17.11153802	-2.02199814	4.74804757	H	21.18257485	-0.00062815	11.72022898
H	8.90500163	-2.02199814	4.74804757	N	18.37497437	-3.29040310	2.00900025	H	22.71802222	0.02780807	9.14600117
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O	12.85742899	-1.60063569	1.03388745	C	20.28567402	-4.12467147	0.50508237	H	23.37806082	0.80597147	10.60795825
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H	10.95100381	-0.57899574	0.97100005	H	17.62793431	-2.78158825	4.26702639	C	24.69525570	-1.37289482	6.77599365
H	12.02521193	-0.09555038	2.02495321	H	19.18363864	-3.52210245	2.58738959	C	24.72843189	0.07853434	7.25489353
N	12.82035059	-2.93796986	1.29598254	H	20.13907626	-5.83377599	-1.35784515	O	25.43202167	0.45287148	8.19624728
C	13.90589258	-3.82343039	0.91997566	H	19.12096480	-4.41298140	-1.71998589	N	23.88863633	0.90149014	6.58176893
C	13.40443125	-4.00000924	1.57600611	C	6.29798669	-6.11072624	1.89507979	H	25.31863968	-4.07978770	6.21176365
O	12.37987689	-5.50954972	0.09635394	C	7.37753832	-6.45621083	2.94905932	H	26.76413729	-2.01949500	6.66217646
C	14.50845819	-4.56385828	2.12768078	O	7.15169092	-6.52980528	4.15185117	H	26.10657788	-1.92470436	8.29608324
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O	13.42530629	-3.08906161	4.48358569	H	5.42299464	-7.06897925	2.35500993	H	23.73118376	1.82758830	6.96267659
N	13.00576287	-4.40034852	4.72771697	N	8.65786982	-6.22724982	2.46439243	C	23.21780701	0.51853429	5.91426422
H	11.99386765	-3.34470601	1.73907395	C	9.74836091	-6.00949850	3.39534532	H	26.30804154	-4.33198213	7.66597523
H	14.68858849	-3.19250303	0.48033794	C	9.90887309	-4.49489656	3.60416922	H	24.60701990	-3.84101820	7.83202093
H	15.43651348	-5.04577310	1.78177934	O	10.33063170	-3.79788734	2.67139391	C	23.25598656	-6.51502296	3.78399241
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H	15.63315855	-4.03760341	3.90682971	O	15.54829590	-8.81449930	2.98261171	C	20.98912823	-3.82366299	3.17140965
H	12.24271357	-4.10093275	3.54641533	N	11.609719165	-7.07374466	1.02430304	H	23.16977020	-4.15700573	5.43714510
N	14.14825015	-4.97509066	-1.22409947	H	8.76984605	-5.93134606	5.11540993	C	23.34100614	-7.52799342	4.17780802
C	13.90699999	-6.01800243	-1.96062016	H	9.48293060	-6.51745125	4.32957290	H	23.55709355	-6.48874386	2.72681523
H	15.04227945	-4.47088181	-1.23888944	C	11.83616812	-6.51029793	3.67309401	C	19.24995609	-5.26295697	-1.04991218
H	13.08999995	-6.62900049	-1.81300313	H	11.46207282	-5.82456952	2.07070878	C	19.50855374	-4.80133050	0.38227257
H	13.66519509	-5.62062255	-1.93905425	C	11.63425033	-9.00851536	0.66821621	H	19.40440520	-3.92134088	1.04830905
H	14.81300107	-6.62200148	-2.23099716	H	12.03892796	-7.26665558	0.58617416	O	17.52936468	-3.48241025	0.28311594
O	16.67539135	-3.04875398	11.34010742	H	9.58042193	-4.04713849	4.81811866	N	18.22106990	-5.83035696	2.82650797
H	17.06780538	-3.90753814	11.18068011	C	9.75202713	-2.59899506	5.11992649	H	19.09509831	-4.38874386	2.72681523
H	16.111505827	-3.24237328	12.10579901	H	10.94641914	-5.61496562	5.46620101	C	19.24995609	-5.26295697	-1.04991218
N	20.72687439	-3.70730495	5.54257076	C	10.66402612	-2.29901398	4.60903811	C	19.50855374	-4.80133050	0.38227257
C	20.99560674	-0.46716165	4.94986949	H	9.85287323	-4.47652721	6.20440967	C	18.44040520	-3.92134088	1.04830905
O	22.15948299	-0.78819212	4.64866337	C	8.90498517	-2.02201507	4.74801168	O	17.52936468	-3.48241025	0.28311594
N	19.96579760	-1.36207280	4.66701787	H	11.66103802	-4.80047116	1.57597691	N	18.61625638	-3.65626060	2.31426962
C	18.63846595	-1.19252439	4.98623985	C	12.84152107	-1.58554985	0.99293556	H	18.37502400	-5.91102470	-1.0960627
O	17.77538802	-2.00561388	4.68509544	O	13.74897829	-1.03871241	0.36632399	C	20.42112853	-4.19129771	0.46653672
C	18.37026972	-0.07558797	5.73101432	H	11.17403011	-4.65065628	2.32204685	H	19.62458109	-5.65036728	1.07085898
N	17.15638823	-0.29389053	6.15176749	H	10.95099831	-0.57900344	0.79100122	H	18.00547826	-2.90035696	2.82650797
C	16.91059942	-1.46620561	6.80486964	C	12.02882346	-0.99476536	2.0198555	C	19.4076240	-3.94868909	2.76549253
C	15.61764308	-1.68116846	7.33315665	H	12.82087840	-2.93489595	1.22083245	H	20.12069990	-5.83091961	-1.39072109
C	15.29208910	-2.83541362	8.01360953	C	13.95293802	-3.78455065	0.91409057	H	19.12100681	-4.41300859	-1.72001020
C	13.93182941	-3.01360944	8.64113930	C	14.3036267	-4.88382519	-0.04329378	C	6.29797213	-6.61098724	1.89505700
C	16.29092926	-3.84554289	18.07072383	H	12.54947418	-6.54190526	0.26551143	C	7.37278753	-6.33678863	2.94175861
C	15.95246601	-5.14116355	8.84960756	C	15.16643549	-3.3365166	3.11665276	O	6.66944757	-7.25648643	1.08473729
C	17.57404703	-3.64561682	6.75735299	C	14.18624836	-2.67043932	4.08990537	H	6.01602178	-5.65100441	1.46297935
C	17.92061844	-2.45203624	6.99020656	H	12.97239486	-2.94025152	4.08357423	C	5.42299744	-7.06901253	2.35498192
N	19.19970087	-2.19410965	6.51790062	N	14.74225209	-1.07198266	4.93675967	N	8.64198254	-6.20718198	2.45261744
C	19.49016636	-0.98911284	5.92166667	H	12.03846254	-3.13312719	1.82640799	C	9.78681757	-5.98529574	3.33035117
C	20.2705204	-3.20235261	3.20928449	H	14.70717462	-3.15636366	0.42413614	C	9.98942435	-4.48184029	3.58847364
H	20.21918444	-2.81428105	4.18347412	H	15.39659251	-5.81074145	1.85226690	O	10.52997097	-3.75067665	2.74403203
H	14.89152135	-0.88043331	7.19049390	H	13.83174717	-3.84891818	2.17659159	C	11.07254207	-6.51235924	2.70669347
H	14.01096010	-3.07291709	7.39616131	C	15.61834238	-2.51257790	2.52361096	C	11.06721114	-8.01539625	2

C	18.42051637	0.13460047	5.49849664	H	11.17400461	-1.45700599	2.33199781	H	19.58557247	-5.60754039	1.07919381
N	17.13497920	0.34834454	5.88073687	H	10.95099947	-0.57899545	0.79100435	H	17.40545169	-3.11721220	2.57780188
C	16.90246427	1.49208954	6.57414899	H	12.02496417	0.09067929	2.03256633	H	18.98901323	-3.82558143	2.72490380
C	15.58580439	1.76095093	7.02712789	N	12.78328025	-2.94777693	1.20158758	H	20.14358036	-5.82892254	-1.35364531
C	15.23562859	2.93211037	7.68933046	C	13.91258498	-3.81449408	0.92310807	H	19.12102618	-4.41299788	-1.72000149
C	13.81949794	3.16060555	8.15667705	C	13.46711150	-4.90148494	-0.05615970	C	6.29800118	-6.10999994	1.89499668
C	16.23405445	3.91320559	7.91838398	O	12.53226862	-5.66920430	0.22477716	C	7.36215667	-6.34234390	2.95074083
C	15.88585371	5.22490186	8.58290244	C	14.49429201	-4.46382387	2.19361754	O	7.09459265	-6.17429292	4.14115265
C	17.55611745	3.65045977	7.51757249	C	14.74974910	-3.44124253	3.32213955	H	6.67182400	-7.25576776	1.08528096
C	17.91555173	2.46070386	6.86452590	C	13.52080982	-3.14511773	4.17578196	H	6.01600072	-5.65100076	1.46300004
N	19.23419449	2.18458378	6.46724323	O	12.97812193	-2.04394971	4.22205267	H	5.42300178	-7.06900163	2.35500070
C	19.51962513	0.98469789	5.82942875	N	13.04977037	-4.72319815	4.88708708	N	8.64340608	-6.26127601	2.48599330
C	20.28896533	3.18766992	6.68785463	H	11.97737584	-3.34311004	4.68757230	C	9.76354086	-6.00233778	3.38531728
C	20.85307592	3.21093468	8.11827915	H	14.69082093	-3.18598961	4.07262925	C	9.92407651	-4.48919992	3.60517472
H	20.34606331	-2.04797430	3.89651084	H	15.44345396	-4.94058368	1.90715993	O	10.37015087	-3.75402385	2.71682025
H	14.83728163	0.99709471	6.80639102	H	13.81481313	-5.25848876	2.53924271	C	11.08082073	-5.61469820	2.80649044
H	13.77790206	3.00024070	9.25083277	H	15.09440907	-2.48154710	2.91334025	C	11.02205527	-7.97166652	2.37613871
H	13.38444417	4.06959229	7.70793966	H	15.54358842	-3.14511773	4.17578196	O	10.58012946	-8.86657717	3.09450670
H	13.17219107	3.21024805	7.89945373	H	12.22880806	-4.09739826	5.46987053	N	11.50243439	-8.18107138	1.12334625
H	16.76962072	5.87224305	8.68188790	H	13.55832674	-5.08408353	4.94218437	H	8.82961064	-6.32702374	1.49164840
H	15.12563450	5.77834965	8.00598536	N	14.13332947	-4.95159355	-1.22618980	H	9.53145959	-6.50799543	4.33189376
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H	18.30866750	4.40997862	7.72412148	H	14.98145465	-3.44904940	-1.29738561	H	11.37821686	-5.87325674	1.96893378
H	19.86823684	4.16589683	6.41055580	H	13.09000588	-6.62900393	8.18299685	H	11.56607097	-9.13271340	0.77852404
H	21.08999921	2.95896555	5.97697437	H	13.66800195	-6.51930453	-3.19269383	H	11.89290825	-7.41122892	0.57967579
H	21.49800280	2.34299822	8.25062893	H	14.81300716	-6.62193976	2.23099760	N	9.59507342	-4.01862808	4.82889026
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H	20.05587293	3.19048446	8.86161944	H	15.91759903	0.30475188	12.34828215	H	9.01735892	-4.60470258	5.42327992
H	12.47283942	-3.67053706	5.13642074	H	16.00810196	1.85319121	11.39328952	H	10.66402029	-2.28999843	4.60900216
AsLOV2 Qe S				N	20.68924740	0.74233854	5.53838973	H	9.84780363	-2.45215783	6.20451990
C	19.02908216	2.11200251	13.81297524	C	21.00048596	-0.49688308	4.99637056	H	8.90500263	-2.02199840	4.74800174
C	19.33212530	0.95045645	12.8959366	O	22.19498015	-0.80677255	4.82890324	C	11.66100659	-0.84000413	1.57600673
O	20.06945882	0.01283509	13.23126948	N	19.98828842	-1.34272386	4.63531336	C	12.85478892	-1.60106875	1.02872546
H	18.15298562	2.65195371	13.45293078	C	18.63326695	-1.16615621	4.96419230	O	13.77921358	-1.05149148	0.42865500
H	18.86981656	1.74089941	14.83433083	O	17.80290349	-2.01290906	4.63104784	H	11.17399651	-1.45700039	2.31199631
H	19.89298778	2.77620040	13.82104795	C	18.35022448	0.05345705	5.71160362	H	10.95102080	-0.57899911	0.79100039
H	18.78062339	1.03836887	11.65987563	N	17.08435297	0.27452966	6.14245640	H	12.0274476	0.09482379	2.04247616
C	18.92685120	-0.02179789	10.65962135	C	16.88208121	1.44019498	6.80762940	H	12.82314550	-2.93150404	1.29708045
C	20.27702616	0.09865453	9.89548988	C	15.62895557	1.67448045	7.40238875	C	13.90846390	-3.82167169	0.91802842
O	20.31994656	0.14617497	8.66262078	C	15.35040846	1.86129297	8.16778855	C	14.30562412	-4.83782156	-0.10743419
C	17.77784933	0.03591492	6.96572577	C	14.03121796	2.96035779	8.86453081	O	12.38222485	-5.50971970	0.09784559
S	16.09649250	-0.26730487	10.37179026	C	16.35044350	3.82317512	8.31197464	C	14.51558743	-4.56602466	2.12358191
H	18.13823216	1.80925454	11.47060967	C	16.08700514	0.50659160	9.12918550	C	14.82805622	-3.61568478	3.29054963
H	18.95396879	-0.97618459	11.19859976	C	17.59713694	3.61809256	7.72442057	C	13.65715466	-3.40051108	4.22358853
H	17.96235201	-0.73324248	8.86933815	C	17.90525145	2.44147048	7.00547719	O	13.42942085	-2.07416188	4.45202342
H	17.72110878	0.98694233	9.17564928	N	19.18073960	2.18482693	6.52417492	N	13.01889721	-4.38310903	4.72842786
H	16.43876664	-0.23095062	11.26860870	C	19.43043850	0.96376225	5.92295250	H	11.99964182	-3.34417795	1.74560483
N	21.35085925	0.12337915	10.71297348	C	20.26030310	3.18418654	8.69766466	H	14.68940977	-3.18957033	0.47661049
C	22.71299149	0.02613231	10.33204026	C	20.85330526	2.21119704	8.11821047	H	15.44212858	-5.04302335	1.77342896
H	21.16741345	-0.03840892	11.70701088	H	20.24570246	-2.21561178	4.14123071	C	13.83290136	-5.35604816	2.46861787
H	22.71799005	0.02709233	9.14600127	H	14.87477813	0.89642607	7.27467129	H	15.17399124	-2.63795356	2.92570349
H	23.15338089	-0.93537345	10.55664242	H	14.99978500	3.03058986	9.95301589	H	15.64180933	-4.03612447	3.90217696
H	23.37804437	0.80596862	10.67099085	H	13.51485959	3.88826353	8.56555030	H	12.25307174	-4.07677438	5.34038906
C	25.51300654	-3.72097468	7.23183700	H	13.36758745	2.10932462	6.86231025	N	14.14804806	-4.95637683	-1.22521758
C	25.85986624	-2.22697099	7.26258197	H	16.962181104	5.76894283	9.05997240	C	13.90700306	-6.01800355	-2.1959806
C	24.68960621	1.37190361	6.77378451	H	15.16855654	5.57447893	8.80743609	H	15.04060571	-4.46787105	-1.24241534
C	24.73243939	0.08190867	7.24506250	H	15.95858055	4.77615640	10.18703372	H	13.09000080	-6.6200028	-1.81000236
O	25.42164387	0.45637321	8.19569763	H	18.35336076	4.38956382	7.85315908	H	13.66510730	-5.62139007	-3.19333614
N	23.91585302	0.91835574	6.55537193	H	19.82986545	4.15704004	6.42318187	H	14.81300208	-6.62201885	2.23100115
H	25.31988251	-0.40829821	6.21269563	H	21.03295972	2.93747956	9.65674502	O	16.80431358	2.95365476	10.80873324
H	26.75873731	-2.05154920	6.65800311	H	21.49782151	2.34285091	8.265092775	H	16.83718745	-3.32259545	9.90738362
H	26.10319284	-1.92151247	8.29286473	H	21.44530802	4.13110161	8.24230370	H	16.27285548	3.58631084	11.31482767
H	23.73721046	-1.77821496	7.16506614	H	20.05581768	3.19799953	8.86185452	N	20.63239620	0.72556684	5.61899379
H	24.58914281	-1.40493319	5.67762700	C	20.91411512	-0.54044713	5.14160161	C	20.2210212568	-0.89166125	5.00508918
H	23.35050889	-1.49170573	5.20428029	C	19.32800407	0.94115794	12.89758686	N	19.88079654	-1.36914965	4.79484265
H	26.30803180	-0.73320203	7.66591992	O	20.06225915	0.00567130	13.24551525	C	18.52265726	-1.12542366	5.01686933
H	24.60697481	-3.84100325	7.81935706	H	18.15294085	2.65193838	6.14350163	O	17.66836250	-1.93779653	4.70655493
C	23.25594873	-6.51500588	3.78413193	H	18.86459985	1.74340784	14.83356279	C	18.26767325	0.12496299	5.77229571
C	21.82271962	-5.96013399	3.94020541	H	19.89301964	2.77579694	13.82116141	N	16.99910495	0.41928953	

C	25.51299474	-3.72098635	7.23815944	H	16.86565824	5.92954935	8.83937275	H	15.58840365	-1.69546968	4.97262880
C	25.83790099	-2.22361665	7.23389697	H	15.25948274	5.90862732	8.07624602	N	14.12981996	-4.95381664	-1.21843836
C	24.66395926	-1.41330356	6.80407974	H	15.46607555	5.23768506	6.9301672	C	13.90706894	-6.01797217	-2.19610229
C	24.59550579	0.03076867	7.17659374	H	18.32924234	4.46307455	7.77904129	H	14.9385796	-4.40551831	-1.27928239
O	25.16213599	0.40491478	8.20942824	H	19.85099804	4.17209149	4.42634264	H	13.09000053	-6.62896657	-1.81294865
N	23.82210213	0.84074635	6.41747315	H	21.03415174	2.93444073	5.96934273	H	13.66729809	-5.61621805	-3.19139726
H	25.31631527	-4.09692887	6.21823665	H	21.49769546	2.34276732	8.25096897	H	14.81297361	-6.62204202	-2.23098706
H	26.75126599	-2.01269104	6.65131695	H	21.45766399	4.12069314	8.26309470	O	17.89584808	3.61616416	10.71411031
H	26.03951567	-1.88314843	8.26228294	H	20.05581716	3.19784586	8.86185119	H	18.51856190	4.35951414	10.69201108
H	23.70776047	-1.87029956	6.99998644	H	12.73809682	-1.97258900	5.12623955	H	17.53796984	3.584544434	9.81050814
H	24.63249047	-1.43409987	5.58023309	<b>AsLOV2 Qa T<sub>1</sub></b>				N	20.61223841	0.70216011	5.61689174
H	23.60316515	6.78655110	7.67818084	C	19.02917980	2.11192613	13.81246776	C	20.88046111	-0.55364780	5.08706239
H	23.20395849	0.43436563	5.7032602	C	19.30611169	0.93423860	12.89847091	O	22.05836135	-0.87162519	4.84700539
H	26.30804466	-4.33201232	7.66590690	O	19.95666966	-0.05647436	13.25628623	N	19.84468808	-1.41225137	4.82171614
H	24.60697074	-3.84100309	7.83194997	H	18.15296144	2.65199946	13.45309635	C	18.50652280	-1.15023194	5.09304335
C	23.25598418	-5.61502963	3.784421042	H	18.86603577	1.74482913	14.83442238	O	17.62863754	-1.95615379	4.76667850
C	21.82313772	-9.61914494	3.94288373	H	19.8927053	7.76036359	13.82127306	C	18.25403122	0.12081241	5.77094794
C	21.67577773	-4.43592857	3.93151174	N	18.79654443	1.06310390	11.64594599	N	16.98137148	0.40350587	6.14991124
O	20.71241764	-3.89270711	3.35893836	C	18.92262853	0.35948523	10.61596512	C	16.80522721	1.61545968	6.72779555
N	22.58396977	-3.69613259	4.59426770	C	20.28111998	0.11336363	9.87731910	C	15.52266179	1.95694392	7.20558498
H	23.91601374	-5.85797310	4.34995587	O	20.34399079	0.14752682	8.64456657	C	15.23862860	3.17661006	7.80943655
H	21.40972043	-2.85895689	4.91595243	H	17.77406375	0.15398063	9.61921888	C	13.85947574	3.47218936	8.31856047
H	21.14144227	-3.64268791	3.17140515	S	16.11285572	-0.18697497	10.32628514	C	16.28258678	4.15586897	7.94862911
H	22.47555432	-2.66794674	4.62675771	H	18.45918663	1.98385095	13.34525578	C	15.99736380	5.49070271	5.85483932
H	23.31721015	-4.12731293	1.51416651	H	18.88631601	-0.29721940	11.1305933	C	17.56296834	3.84068814	7.50292068
H	23.34101820	-7.52802194	4.17694426	H	17.90981074	-0.56659440	8.80362227	C	17.86819461	2.59245048	6.91112954
H	23.58400206	-6.49765139	2.73388735	H	17.78035837	-1.15322774	9.16235174	N	19.14811947	2.26049128	6.51673834
C	19.25001906	-2.63206236	-1.05000492	H	16.22455429	0.66372038	11.37935993	C	19.36806305	0.98416370	5.96137057
C	19.35420284	-4.76495577	0.39059470	N	21.34814547	0.1511623	10.70478036	C	20.27273994	3.20538656	6.69396647
C	18.06813972	-4.07296468	4.86226302	C	22.71316527	0.02574816	10.23649646	C	20.85341935	3.21125106	8.11804960
O	17.08298473	-3.92919684	0.12332881	H	21.15697177	-0.04281421	11.69578835	H	20.08181516	-2.34351925	4.42146540
N	18.10920568	-6.35591429	2.14416035	H	22.71792792	0.02721948	9.14599985	H	14.74301558	1.20409835	7.08062361
H	18.37499850	-9.51099438	-1.09610127	H	23.14781353	-0.93712061	10.55967946	H	13.88131171	3.68272421	9.40138560
H	20.18937604	-4.05805939	0.53108034	H	23.37790948	0.80625108	10.60763842	H	13.44398900	4.37255517	7.83532258
C	19.56100827	-5.59756370	1.08584953	C	25.51286287	-3.72105587	7.23796317	H	13.17433601	2.63302983	8.14219506
H	17.38234427	-3.0659171	2.532287306	C	25.85195689	-2.22590265	7.24427355	H	16.89330982	6.12726203	8.60235547
H	19.85582413	-2.60896937	2.69678005	C	24.69779716	-1.38611669	6.73179132	H	15.20604965	6.03182613	8.04010401
H	20.14650532	-6.78084677	-1.34702279	C	24.69507578	0.06299593	7.19089453	H	15.64415205	5.37100355	9.62229742
H	19.12098956	-4.41991187	-1.71998682	O	25.38127712	0.46155706	8.14222448	H	18.34710043	4.58690869	7.61838425
C	6.29799647	-6.61100021	1.89502055	H	23.86023787	0.88846276	6.50571632	C	19.90233231	4.19692537	6.40152248
C	7.36217805	-6.38435202	2.95124682	H	25.30236081	-4.09136722	6.21942412	H	21.03973017	2.91555907	5.96994785
O	7.09371892	-6.17591215	4.14159456	H	26.75516393	-2.01667905	6.64499974	H	21.49780923	2.34282705	8.25079842
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H	5.42300130	-7.06900280	2.35499867	H	24.60177977	-1.42080060	5.63321771	<b>AsLOV2 Qb T<sub>1</sub></b>			
N	8.64391499	-6.26534025	2.48775894	H	23.71435069	1.82423576	6.88667262	C	19.02901141	2.11201205	13.81290333
C	9.76314043	-6.00380212	3.38740741	H	23.19035107	0.50542340	5.83940099	C	19.33210911	0.93856719	12.90627088
H	9.92072717	-4.48951572	3.60586501	H	26.30805567	-4.33195540	6.76569326	O	20.06186592	-0.00097711	13.25215134
O	10.36285108	-4.37234953	2.73783736	H	24.60701638	-4.75722040	6.25520040	H	18.15302505	2.65220040	13.45295522
C	11.08211022	-6.51159992	2.80951961	C	23.25608266	-6.51499565	3.78043616	H	18.86662469	1.74736360	14.83617216
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O	10.58626807	-8.86380719	3.10473736	C	21.63706773	-4.46303098	3.97165488	N	18.78025397	1.01676896	11.66919338
N	11.52644967	-8.18741715	1.13869339	O	20.48060329	-3.99102507	3.90847446	C	18.92895262	-0.01994943	10.65069022
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H	11.37636384	-7.23873397	1.96980886	H	21.16659163	-6.33685237	3.10867159	S	16.11318386	-0.27850751	10.39468374
H	11.59680961	-9.17372249	0.80009384	H	22.54263108	-6.26344946	4.29165296	C	18.22339049	1.84077326	11.41839803
H	11.91643108	-7.41571823	0.59428659	H	23.63679257	-4.02205495	4.21820774	H	18.92852007	-0.99455676	11.16795897
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C	9.75200077	-2.59005976	5.11999444	H	23.60063875	-6.50903421	2.73823519	H	17.75764619	1.05515210	9.19452910
H	9.01835578	-6.40455475	5.42628389	C	19.24991836	-6.51685962	1.07780757	H	16.45402386	0.00124586	11.67984731
H	10.66446014	-7.23899971	4.60900031	H	23.34604336	-7.47715718	0.38799789	H	22.71316898	0.12548785	10.71361061
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C	11.66100415	-8.04008848	1.57601001	N	10.61594391	-8.86878923	3.23549312	C	20.74551461	-0.03768020	11.70727079
C	12.85205768	-6.16015916	1.02236365	H	18.29043694	-3.34980773	2.12019324	H	22.71792940	0.02805125	9.14600127
O	13.70045035	-6.30109924	1.41343308	H	18.37510333	-6.11360926	1.09602224	C	23.15368464	-0.93575532	10.55656572
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H	8.83577508	-6.34965089	1.49646538	N	22.72204032	-3.64411822	4.15328676	C	20.27513964	0.08739338	9.89679769
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H	11.82916245	-6.52757953	3.62937700	H	21.38348056	-6.23967764	4.86569584	C	17.76537895	0.02375577	9.66902594
H	11.42100486	-5.88180586	2.03114021	H	21.15895430	-6.353341821	3.12598701	S	16.10545819	-0.28818806	10.39711303
H	11.29483736	-9.04361871	0.60403812	H	22.58573436	-6.28868130	4.22677157	H	18.21306925	1.83360715	11.42965606
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N	9.61241493	-4.02667627	4.84237100	H	23.34098894	-7.52801040	4.17697796	H	17.90943560	-0.73878770	8.89418016
C	9.75200400	-2.59914533	5.11997549	H	23.60696242	-6.51073847	2.74011741	H	17.75055109	0.99134369	9.15135962
H	9.00391115	-4.60005001	5.41985339	C	19.25003991	-5.26304835	-1.05004885	H	15.97991941	0.92151250	11.00017348
H	10.63596341	-2.28990025	4.60898335	C	19.34606695	-4.76299136	0.3928809	N	21.35116469	0.12064689	10.71455673
H	9.85078308	-2.44468221	6.20324104	C	18.04513850	-4.09978704	0.86642056	C	22.71303393	0.02595786	10.23613064
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C	11.66102124	-0.83998800	1.57601336	N	18.05116711	-3.72965600	2.16325056	C	22.71797925	0.02798958	9.14600133
C	12.85418846	-1.60131920	1.20940723	H	18.37498781	-5.91092853	-1.09597989	H	23.15631111	-0.93520372	10.55455753
O	13.79028412	-1.05517518	0.44457768	H	20.16275430	-4.02524605	0.52645314	H	23.37800499	0.80604208	10.60790925
H	11.17399376	-1.45700348	2.33199217	H	19.57482695	-5.59049897	1.08716243	C	25.51300760	-3.72100054	7.28304244
H	10.95099492	-0.57901422	0.7910193	H	17.30753427	-3.15244396	2.53745125	C	25.84927587	-2.22565698	7.23704769
H	12.02782733	0.02941945	2.02801722	H	18.87551170	-3.87140618	2.74530226	C	24.67266873	-1.38992963	6.72756668
N	12.80202751	-2.94162528	1.27687555	H	20.14863559	-5.82610382	-1.34294373	C	24.70346589	0.07271256	7.16986626
C	13.88886889	-3.83386609	0.93290888	H	19.12099162	-4.41298365	-1.71997763	O	25.36954801	0.46405029	8.12918481
C	13.39581450	-4.84633986	-1.02050766	C	6.29798826	-6.46109823	1.89509072	N	23.90772285	0.89761134	6.44107658
O	12.36399650	-0.59352657	0.99315730	C	7.35471549	-6.34957945	2.95885703	H	25.30299196	-4.09671365	6.22123825
C	14.44595183	-2.05840081	2.15726859	O	7.07542685	-6.17402220	4.15457877	H	26.74858747	-2.01707441	6.63161801
C	14.78797311	-3.65179502	3.33254272	H	6.67390478	-7.25575326	1.08635819	H	26.08531829	-1.89712059	8.2618647
C	13.62983377	-3.28092693	4.22530202	H	6.01599172	-5.65100140	1.46300472	H	23.72290420	-1.79782857	7.12285457
O	12.96253299	-4.39786881	4.65216609	H	5.42300501	-7.06902095	3.53498988	H	24.57602577	-1.44587172	5.63144406
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H	15.24478791	-2.71420465	2.98708877	C	10.98551506	-3.08481885	2.45147553	C	21.82876134	-5.95695316	3.90128760
C	15.52423715	-4.15753114	3.98030404	O	10.51732035	-8.91189231	3.16617860	C	21.66345631	-4.43802044	3.88720943
H	12.60780137	-0.21905195	3.22618015	N	11.46946654	-2.025103433	1.20152703	O	20.53795621	-3.94235646	3.67325937
N	14.14665225	-4.96418363	-1.21443543	H	8.84089773	-6.34178821	1.51767251	N	22.71537120	-3.65093636	4.16305497
C	13.90701036	-6.01802143	2.19596484	H	9.48530787	-5.61809372	4.37687544	H	19.31599902	-5.85801030	4.35001628
H	15.04376850	-4.48375516	-1.21831227	H	11.81702249	-6.51150319	3.69787787	C	21.37551330	-6.26751448	4.86009920
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H	13.66573623	-6.51624513	3.19035378	H	11.51130970	-9.20414044	0.85794511	H	22.57295722	-2.63900814	4.26314326
H	14.81300502	-6.62199646	-2.23104157	H	11.90623172	-4.96095784	0.67235954	H	23.62879130	-4.03046529	4.37011420
O	16.83359931	-2.98110383	10.82625354	N	9.59220184	-4.02434400	4.83826507	H	23.34099857	-7.52800659	4.17698086
H	17.05902654	3.31109968	9.94072004	C	9.75198765	-2.59819279	5.11999028	H	23.60572113	-6.51011759	2.73971754
H	16.18513953	2.27535439	10.63942726	H	8.97996472	-4.59570692	5.41496019	C	19.24998855	-5.26300084	-1.04997761
N	20.71191275	0.71883458	5.59213100	H	10.66403411	-2.29001800	4.60909745	C	19.35441684	-4.76323162	0.39160680
C	21.02262563	-0.56105150	5.03395800	H	9.85240581	-4.22448306	6.20345071	C	18.06510791	-4.07916839	0.86525455
O	22.21409856	-8.81458478	4.84105711	H	8.90498326	-2.02206730	4.74793713	O	17.08710776	-3.92090203	0.12178569
N	20.01197228	-1.37486696	4.69328095	C	11.66099632	-0.83999238	1.57599970	N	18.09642837	-3.67312086	2.15192784
C	18.66592935	-1.19409362	5.01937486	C	12.85893730	-1.59534281	1.03441046	H	18.37500940	-5.91100862	-1.09620222
O	17.82398242	-2.03864760	4.69441593	O	13.82294002	-6.02722262	0.50889040	H	20.18376969	-4.04669171	0.52304494
C	18.37960012	0.04357269	5.75169615	H	11.17400434	-1.45700692	3.23319968	O	19.05912443	-5.59470350	1.08637849
N	17.10190302	-6.02180243	5.15668833	H	10.95100138	-6.58209982	0.79100150	H	17.33575592	-3.13132518	2.54344832
C	16.87781736	1.47326611	6.72339179	H	12.02515965	0.09065672	2.02343694	H	18.90766964	-3.85086960	2.74286436
C	15.57342180	1.77065590	7.18232738	H	12.78007444	-2.94897734	1.20160801	H	20.14674997	-5.82756461	-1.34590240
C	15.23476610	2.98760343	3.75824357	C	13.90831478	-3.81728130	0.92455974	H	19.12099977	-4.41297970	-1.71996463
C	13.83349647	3.24940877	8.23029000	C	13.46364628	-4.90219049	-0.05711767	C	6.29796562	-6.61009990	1.89500084
C	16.24137853	2.24548765	7.90519583	O	12.56224430	-5.66822476	0.523036979	C	7.36156415	-6.34251446	2.95114534
C	15.89116416	5.33996027	8.50913183	C	14.48489747	-4.46495878	2.19593810	O	7.09363404	6.17508124	4.14152705
C	17.54327188	3.70350855	7.49410475	C	14.74036573	-4.43946344	3.32628288	H	6.67203376	-7.25579803	1.08541038
C	17.89975436	2.49439709	6.90933933	C	13.51134749	-3.15161689	4.17944253	H	6.01600172	-5.65100188	1.46229928
N	19.19182316	2.21020624	5.15335031	O	12.97002325	-2.04987925	4.22366614	H	5.42300522	-7.06900317	2.35500060
C	19.45807610	0.95109065	5.94417993	N	13.03875675	-4.21760503	4.88943339	N	8.64276599	-6.26105153	2.48659891
C	20.27712024	3.19699452	6.69454687	H	11.97279581	-3.34332738	1.68621688	C	9.76285245	-6.00311363	3.38613697
C	20.85323991	3.21131979	8.11815193	H	14.68868697	-3.18964404	0.47650797	C	9.92325080	-4.48992928	3.60553957
H	20.26754690	-2.24548790	4.18966192	H	15.43320999	-4.95020931	1.91245385	O	10.36949040	-3.75513251	2.71656684
H	14.82641377	0.98668602	4.07240526	H	13.80237016	-2.26463853	2.53973005	C	11.07937454	-6.51742003	2.80722251
H	13.82021291	3.02837803	9.30733916	H	15.08606659	-2.48881079	2.930236808	C	11.01720060	-7.97533103	2.37445065
H	13.39657947	0.37161611	7.71339801	H	15.53219651	-3.82878908	3.99337673	O	10.57510656	-8.86897233	3.09198914
H	13.18439026	3.27640175	0.58598627	H	12.22258561	-4.09391422	5.47934794	N	11.49455245	-8.18163591	1.11910868
H	16.76167222	0.01021164	5.83325244	H	13.55321023	-0.02851176	4.95571733	H	8.82912465	-6.32676847	1.492

C	15.28970214	3.03756581	7.92182162	C	13.36658106	-4.80523874	-0.12637054	C	6.29800414	-6.61100804	1.89500984	
C	13.94243423	3.27314036	8.53759466	O	12.30629173	-5.42681027	0.04049965	C	7.36222298	-6.33568130	2.94726510	
C	16.29884871	4.06162524	7.99354086	C	14.48983644	-4.62355864	2.10219034	O	7.09891840	-6.15808227	4.13707754	
C	15.97236371	5.41747553	8.56405237	C	15.06827226	-3.72523733	3.19718728	H	6.67275524	-7.25572378	1.08581752	
C	17.57769624	3.78011551	7.52111305	C	14.10058731	-3.34162095	4.31447785	H	6.01600648	-5.65100198	1.46299472	
C	17.90249513	2.53506188	6.93513572	O	12.93502897	-3.72723872	4.37225555	H	5.42299485	-7.06899158	2.35499791	
N	19.18104456	2.23139457	5.51319047	N	14.65117375	-5.21708588	5.25634229	N	6.4319626	-6.25397389	2.47933097	
C	19.41733369	0.96611472	5.93903686	H	12.07322037	-3.30640115	1.89733251	C	9.76100441	-6.00762797	3.38295452	
C	20.28460472	3.19720078	6.69073547	H	14.69407833	-3.20938846	0.48975169	C	9.93023084	-4.49494941	3.60544580	
C	20.85331246	3.21123256	8.11819470	H	15.29303040	-5.25276255	1.69186758	O	10.37726814	-3.76164988	2.71860491	
H	20.15256367	-2.28623538	4.25778177	H	13.71956064	-5.28168495	2.52897506	C	11.07878699	-6.54149754	2.81195238	
H	14.83951418	1.03674694	7.24891015	H	15.46056914	-2.78793112	2.76491092	C	10.94686501	-7.96218102	2.28052554	
H	14.05424716	3.40181955	6.92867210	H	15.92838119	-4.21980765	3.67759906	O	10.58068404	-8.90396126	2.97965433	
H	13.47425984	4.19435446	8.15487414	H	14.12441511	-3.29174887	6.11467873	N	11.23866176	-8.07158397	0.95719753	
H	13.26276992	2.42982066	8.35931854	H	15.66401461	-2.39359355	5.29195834	H	8.83350496	-6.34864694	1.48774067	
H	16.86232157	6.06088251	8.607834022	H	14.14577725	-4.96708251	-2.11682845	H	9.51711995	-6.50964853	4.32867629	
H	15.21308485	5.93092775	7.95023585	C	13.90706502	-6.01798598	-2.19610388	C	11.83001670	-6.53387601	3.61589601	
H	15.54967735	5.34497004	7.95036928	H	15.05055107	-4.49537236	-2.11033743	H	11.42841324	-5.86382543	2.02484934	
H	18.33957828	5.24531714	7.608363669	H	13.09000281	-6.62896355	1.81294032	H	11.24606331	-8.99771851	0.54336988	
H	19.89905067	4.18191084	6.39365764	H	13.66362888	-5.61866999	3.19201061	H	11.65066234	-7.28668991	0.45083404	
H	21.06195371	2.91945340	5.97317318	H	14.81298054	-6.22203302	-2.23100011	N	9.61242816	-4.02556414	4.83704759	
H	21.49781082	3.24824746	8.25093421	O	17.85946132	3.58689550	10.68128280	C	9.75199892	-2.591912814	5.11997460	
H	21.45081189	4.12604723	8.25685014	H	14.9868902	3.61335629	10.67771620	H	9.00425591	-4.60154978	5.41232690	
H	20.05581282	3.79198327	8.86184907	H	17.51581584	3.57365260	7.79151921	H	10.63697828	-2.28994756	4.60897590	
H	12.74432375	-1.99817247	5.16152446	N	20.65037515	6.69094238	5.60941383	H	9.84937044	-2.44770166	6.20373799	
AsLOV2 Qs T <sub>14h</sub>	C	19.02910952	2.11196333	13.81254804	C	20.88521692	-0.53799531	0.58061306	H	8.90503205	-2.02193450	4.74803811
C	19.30642221	0.98436564	12.89792237	O	22.04105257	-0.90591060	4.79289557	C	11.66102334	-0.833998455	1.57601361	
O	19.97257858	-0.04676362	13.25520893	N	19.82674908	-1.42137828	4.86228105	C	12.85911129	-1.59563486	1.03333093	
H	18.15298324	2.65200875	13.45306111	C	18.51074617	-1.5049275	5.15003033	O	13.78771629	-1.04890276	0.43962902	
H	18.86528042	1.74426713	8.183417134	H	17.58581667	-1.94795616	4.99025887	H	11.17399402	-1.45700460	2.33199143	
H	19.89300551	2.77599239	13.82125348	C	18.30777886	0.14744754	5.75490329	H	10.95099529	-0.57901480	0.79100138	
N	18.78717138	0.50800417	11.65023153	N	17.04597661	5.18866533	6.11033138	H	12.02270141	0.09570114	2.02656833	
C	18.92465237	0.07173358	10.63297850	C	16.78780839	1.73647014	6.69823344	N	12.82485395	-2.93346496	1.30500159	
C	20.2859173	0.08852485	9.89041412	C	15.49272750	-0.79237437	7.11453141	C	13.90399087	-3.82389957	0.93196942	
O	20.34288502	0.09569437	8.65787855	C	21.51950281	3.30356858	7.71607105	C	13.39577825	-4.82705616	-0.10806488	
C	17.78730790	0.11709974	6.91695046	C	13.82591209	3.64126723	8.17515475	O	12.349778703	-5.46862437	0.08207450	
S	16.11561178	-0.14411713	10.27697963	C	16.28553784	4.22348951	7.89547373	C	14.47805537	-4.58650604	2.14124529	
H	18.40572052	0.95120120	11.35223706	C	16.03698620	5.56198023	8.54428432	C	14.85604086	-3.66360546	3.31283542	
H	18.88871657	-0.24887233	11.15151007	C	17.57969886	3.87332048	7.48812150	C	13.73159159	-3.27108645	4.24036077	
H	17.94016434	-0.60649568	8.80360185	C	17.87101501	6.32642738	6.89241201	O	12.95699495	-4.34879681	4.56597055	
H	17.79702005	1.10234743	9.12483524	H	19.16715689	2.26934270	6.49673660	N	13.60623099	-2.08137242	4.68897127	
N	21.35209287	0.13525658	10.71611129	C	19.41370030	0.10181080	5.95156434	C	11.99304975	-3.33676309	1.73776450	
C	22.71324327	0.02572858	10.23641830	C	20.28558592	4.21254539	6.89852223	H	14.70057276	-3.20115827	0.50580521	
H	21.16697624	-0.28548243	11.70812199	C	20.85344526	3.21127845	8.11804848	H	15.38167357	-5.10699933	1.79249749	
H	22.71791030	0.02788896	9.14600032	H	20.05675089	-0.235962104	4.791510108	H	13.7617551	-5.34770832	2.48059123	
H	23.15116274	-0.39686431	10.57451450	C	14.69204661	1.35173721	6.96662827	H	15.32366157	-2.73378540	2.96082300	
H	23.37788444	0.80626410	10.60769764	C	13.80319467	3.83836593	9.25987874	H	15.60043709	-4.18279195	3.94076770	
C	25.51285392	-3.72113307	7.23795660	H	13.45125074	4.55224747	7.68004879	H	12.82757899	-2.02166607	5.36139189	
C	25.84449608	-2.22504139	7.22884861	H	13.12327430	3.72113307	7.96232949	N	14.15302222	-4.96411735	1.21359150	
C	24.67226375	-1.40404406	6.68756344	H	16.95531860	6.16405927	5.98403390	C	13.90701266	-6.01802021	2.19599797	
C	24.66551250	0.05555542	7.130600617	H	15.27969551	6.13963261	7.98966225	H	15.05572542	-4.49375172	1.21562845	
O	25.33001048	0.46969996	8.08356216	H	16.35466167	5.43916973	9.57131876	H	13.08988482	-6.62899229	1.81301677	
N	23.84039252	0.85722154	6.40562329	H	19.92195626	4.2095056	6.39842055	H	13.66507931	-5.61310527	3.18963378	
H	25.30106269	-0.40984633	6.22194380	C	21.05976503	2.92486825	9.79159898	H	14.81300444	-6.62199783	2.23101069	
H	26.75378923	-0.21913603	6.63751643	H	21.49776557	3.24794273	8.25080324	O	16.82046323	2.98908814	10.91145116	
H	26.06098604	-1.88419447	8.25393305	H	21.45522835	4.12233686	8.26644004	H	16.22464449	2.22052212	10.79916571	
H	23.71562968	-1.82640439	7.04895640	H	20.05569073	3.19807387	8.816812801	N	12.76909707	0.71998892	5.57407543	
H	24.60858298	-1.45749745	5.58894420	H	16.29043596	-0.27131864	5.89132613	C	21.05841336	-0.47853184	4.98696383	
H	23.65818794	1.78674746	6.76716920	C	17.82395803	0.86320620	9.14705571	O	22.23248913	-0.82632333	4.76327162	
H	23.16967509	0.44668249	5.75557595	C	19.02899781	2.11200839	13.81289280	N	20.0267542	-1.34855140	4.61948285	
H	26.30806106	-4.33194951	7.66596167	C	19.32946397	4.93439758	12.89901046	C	18.69565943	-1.15390276	4.91914211	
H	24.60706567	-4.77100156	7.83209745	O	20.04838310	-0.00580083	12.34208306	C	17.79657268	-1.9482058	4.61306887	
C	23.25606779	-6.51499152	3.78402003	H	18.15302960	2.65200961	13.45295178	C	18.44707291	0.08224617	5.63240865	
C	21.81974658	5.98360430	9.316664840	H	18.86724886	1.74274883	14.83446805	N	17.1686715	0.36277714	6.00626460	
C	21.61030358	-4.47426013	3.98107398	H	19.89301921	2.77597480	13.82111934	C	16.85070221	1.53713379	6.64921522	
O	20.44252433	-0.42250237	4.19047969	H	18.8995812	-0.97951704	11.42218932	C	15.53860304	1.7945198	7.07511204	
N	22.65719102	-3.65216021	4.13552646	C	18.24023145	0.0699688	9.89321595	C	13.79088744	3.22919307	8.18634706	
C	21.36154937	-6.35211331	3.11058709	H	22.71317443	0.25815893	10.23616224	C	16.21472758	3.95187350	7.93207427	
C	21.16575754	-2.01973307	7.23795660	C	17.79663449	0.08776833	6.909					

N	23.92949929	0.86552777	6.26296763	H	19.84043730	4.17950923	6.42972350	H	14.81300229	-6.62200159	-2.23099982
H	25.30184645	-4.10902466	6.22553676	H	21.04655794	2.96898490	5.96219720	O	16.33533416	2.83185216	11.65682212
H	26.74250939	-2.02024260	6.1405509	H	21.49785183	2.34285641	8.25094675	H	15.87149264	2.96823667	12.49760756
H	26.05417590	-1.86962808	8.23250968	H	21.44760179	4.12861007	8.25309007	H	16.04088454	1.94064089	11.36540061
H	23.70894176	-1.82046294	7.06449812	H	20.05581890	3.19795723	8.86185511	N	20.76811492	0.74278108	5.51527749
H	24.57376783	-1.50490875	5.57091905	H	16.43259080	-0.32101577	5.82982552	C	21.05438064	-0.45047849	4.91600855
H	23.74644090	6.08655120	6.59400705	<b>AsLOV2 Qd T<sub>1,ii</sub></b>				O	22.23185835	-0.79768834	4.69050999
H	23.28884879	0.46009536	5.57512944	C	19.02908079	2.11202760	13.81285914	N	20.02565490	-1.31085460	4.54206258
H	26.30802619	-4.33200333	7.66595522	C	19.32202648	0.95679346	12.88473305	C	18.69743884	-1.13473002	4.86168178
H	24.60698121	-3.84100017	7.83196749	O	20.03298591	-0.02077480	13.21248406	O	17.79837633	-1.93359007	4.56456682
C	23.25602768	-6.51499613	3.78402454	H	18.15297514	2.65196765	13.45302025	C	18.45116287	0.08960301	5.59308977
C	21.83230138	-4.20232552	3.89863912	H	18.87155432	1.73402478	14.83168934	N	17.18093364	0.34146391	6.01318385
C	21.67445504	-4.42627998	3.83830436	H	18.92997778	2.77606013	13.82110013	C	16.88178074	1.45865461	7.5913062
O	20.55983001	-3.93386892	3.56718963	N	18.79014144	1.07835032	11.64133469	C	15.61896564	1.62393728	7.34685763
N	22.71595017	-3.63257035	4.13309485	C	18.91476072	0.36881464	10.62709309	C	15.32904622	2.72648669	8.15501289
H	23.91599432	-3.85798733	4.34999478	C	20.28439072	0.10320197	9.88502646	C	13.99228992	2.85809659	8.83380734
H	21.38870759	-6.22389606	4.87113602	O	20.34616967	0.12473862	8.65388665	C	16.32549739	3.72212386	8.32943240
H	21.15680556	-6.35765406	3.13299495	C	17.80782576	0.14642805	9.57217602	C	16.05061464	4.94027516	9.16972588
H	22.57322102	-6.41528624	4.19596066	S	16.09652118	-0.03624997	10.16093260	C	17.58206343	3.54776196	7.74617191
H	23.61978629	-4.00991719	4.38455806	H	18.16260421	1.86251235	11.46495457	C	17.91141901	2.41084068	6.98425787
H	23.34098762	-7.52800807	4.17694823	H	18.87394486	0.93622582	11.44233509	N	19.20432863	2.18990598	6.48768106
H	23.60659501	-6.51081716	2.73959373	H	18.01303872	-0.57453735	8.77316341	C	19.51346784	0.99095020	5.8590305
C	19.25003372	-5.26305493	-1.05004727	H	17.86474129	1.15522592	9.12695650	C	20.25985393	3.20502413	6.69851903
C	19.34710462	-4.76437965	0.39222758	N	21.35003812	0.79021515	10.71036963	C	20.85328123	3.21115595	8.11823089
C	18.04743228	-4.02166046	0.86738000	C	22.71305505	0.02593953	12.3613482	C	20.29023424	-2.18545045	4.04295093
O	17.07763686	-3.92008062	0.11685334	H	21.16039767	-0.02795448	11.70613974	H	14.86201561	0.85620105	7.17473209
N	18.05574639	-3.74035695	1.26885540	H	22.71797195	0.02799533	9.14600133	H	14.1294775	2.96964044	9.92139560
H	18.37498749	-5.91091898	-1.09598299	H	23.15177405	-0.93609148	10.55761471	H	13.45104473	3.75333626	8.48466328
H	20.16335666	-4.03519151	0.52631440	H	23.37800081	0.80604395	10.60791280	H	13.35756128	1.98005363	8.65080433
H	19.57778880	-5.59209233	1.08601002	C	25.13004447	-3.72100197	7.23803831	H	16.87442624	5.66524944	9.10545995
H	17.32408476	-3.14903664	2.54472048	C	25.85530685	-2.22672247	7.25078899	H	15.12274953	5.44664261	8.85871132
H	18.88643391	-3.88203496	2.74289675	C	24.68324862	-1.38285173	6.74776220	H	15.93500073	4.63812407	10.22258619
H	20.14823669	-3.82623537	-1.34381402	C	24.70570801	0.07185209	7.21689106	H	18.3059375	4.31716405	7.91705929
H	19.12099443	-4.41298233	-1.71976633	O	25.37191963	0.44704285	8.18519362	H	19.81827938	4.17995308	6.44549208
C	6.29798662	-6.61098118	1.89500538	N	23.90477031	0.90068525	6.50506009	H	21.03876987	2.99214118	5.95927598
C	7.35434253	-6.34235039	2.95627571	H	25.31829127	-0.80839738	6.21472836	H	21.49785088	3.24287636	8.25092854
O	7.07751350	-6.16548415	4.14342822	H	26.75645522	-0.21084937	6.48461018	C	21.44716894	4.12882446	8.25333535
H	6.67543600	-7.25562706	1.08712340	H	26.09162033	-0.99082892	8.27926196	H	20.05582049	3.19802400	8.86185802
H	6.01599066	-5.65100129	1.46300559	H	23.7099368	-1.79581763	7.13243462	H	12.98656898	-1.94460392	5.28997657
H	5.42300543	-7.06902009	2.35499070	H	24.59155707	-1.94179783	6.56059583	H	16.47569081	-0.35780606	5.78159335
N	8.64213510	-6.27349029	2.50514389	H	23.75415159	1.83572696	6.86597178	<b>AsLOV2 Qd S<sub>1</sub></b>			
C	9.74744530	-6.03283601	3.42536430	H	23.25923958	0.52822731	5.80609129	C	5.51900438	-6.15600101	1.90999832
C	9.94068358	-4.51857107	3.62616793	H	26.30801233	-0.43320075	7.65695742	C	6.63037349	-5.97617425	2.93725172
O	10.42285798	-3.81661992	2.73174394	H	24.60699661	-3.84090909	7.31919188	O	6.41029703	-5.91322978	4.14650171
C	11.06571885	-6.03583231	2.89255068	H	23.25602662	-6.51500682	3.78385260	H	5.85396320	-6.71152192	1.02131968
C	10.91212860	-6.02503697	2.36172423	H	21.82732108	-5.94941658	3.94046805	H	5.1899864	-5.16600058	1.59400125
O	10.50012976	-8.95212899	0.52539303	C	21.70879294	-0.42297667	3.94237887	H	4.6849996	-6.67599952	2.38200056
N	11.24117424	-8.15099718	1.04935474	O	20.75943763	-3.85174310	3.36825705	N	7.89113514	-5.8712864	2.42283092
H	8.84266724	-5.12521585	1.51426323	H	22.62779824	-0.49813725	6.21405487	C	9.07268710	-5.76323151	3.27186679
H	9.47253713	-6.51541820	4.37236711	H	23.91599109	-5.85803033	4.35004861	C	9.48466963	-4.28517502	3.43659119
H	11.78505781	-6.63085240	3.72530113	H	21.40456788	-0.80839738	6.21472836	O	10.11483385	-3.69318288	2.55270851
H	11.46535108	-5.93394902	2.119414145	H	21.14423405	-6.31607634	3.16150142	H	10.22812488	-6.57143255	2.68934274
H	11.23333654	-9.07996874	0.64188056	H	22.55132176	-2.68099601	6.43919797	C	11.32283803	-6.80177998	3.73194243
H	11.69730530	-7.38468667	0.52539303	H	23.34792164	-0.15375752	5.16171748	H	11.06321770	-6.94256693	4.92693586
N	9.59422245	-4.02521589	4.83763978	H	23.34099725	-7.52729680	4.17078617	N	12.57321297	-6.89019455	3.21818432
C	9.75190935	-5.18907748	1.51998588	H	23.58542565	-6.49813760	4.32174011	C	8.02198017	-5.84260411	4.18001051
H	8.96802949	-4.59014466	5.04017222	H	19.24994773	-5.26229851	-1.04998482	H	8.80111048	-6.1795676	4.24954963
H	10.66403236	-2.29001745	3.62616793	H	19.36968308	-4.77381889	4.89960999	H	10.63671211	-6.07604254	1.79754096
H	9.85209523	-4.82753653	6.20356759	H	18.09095885	-4.08407909	4.87721036	H	9.84740228	-7.56324175	2.39345398
H	8.90498231	-2.02206724	4.74793939	O	17.10200415	-0.92096938	1.048448132	H	13.34210603	-6.98202961	3.87329518
C	11.66099240	-8.95119941	1.57600783	N	18.14178093	-3.68867108	2.166399020	H	12.75837510	-6.54389624	2.72224398
C	12.86566579	-5.18907798	1.04981833	H	18.37502555	-5.91103428	3.10962321	C	9.10168104	-3.70965699	4.59541115
O	13.81566330	-6.01774793	2.19062782	H	20.0720908	-0.46823563	5.02532910	C	9.35900745	-2.30799658	4.90300893
H	11.17399990	-1.45700907	2.33199225	H	19.58244006	-5.61123261	1.07766440	H	8.47034861	-4.23811289	5.18883285
H	10.95100413	-5.07899406	0.79100057	H	17.42081101	-0.30656454	5.55943686	H	10.27627604	-2.00352368	4.38304221
H	12.01850789	-0.09327407	2.03320272	H	18.99507601	-3.81705954	2.70834358	H	8.52600059	-1.68400265	4.57999444
N	12.79115954	-2.94086680	1.21602394	H	20.14249819	-0.94086680	1.35611720	H	9.5229725	-2.18499825	5.97400082
C	13.30908475	-3.81283663	0.92041470	H	19.12102015	-4.41303668	3.11999464	C	18.97700054	2.1999730	13.59599664
C	14.44621419	-4.88181108	-0.60578087	H	19.011108	-4.60578087	5.41988583	C	19.10180335		

H	18.19301053	-5.85401316	-0.88000367	H	23.16600130	0.83900024	10.27400105	O	11.69624572	-5.65846835	4.29356853
H	20.12767339	-4.04669789	0.67282837	H	22.84869820	-0.91792962	10.41953004	N	12.53204022	-7.24489354	2.89367349
H	19.48672893	-5.57430890	1.26004686	C	25.39799383	-3.82699914	7.28699763	H	8.00326412	-5.76845170	1.37030578
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H	18.39301799	-4.37400854	-1.52501394	C	24.73881324	0.00801351	7.27937197	H	9.98637999	-7.48635791	2.29872883
H	19.95110478	-5.08183654	-1.19021164	O	25.54061864	0.41261647	8.12066167	H	13.45298221	-7.07842819	3.28996287
C	11.32700414	-0.63299703	14.3000718	N	23.85844724	0.82850840	6.64283360	H	12.52969147	-7.49902017	1.90993498
C	12.57482235	-1.36188667	0.95499377	H	25.19601069	-4.16200548	6.27000040	N	9.11154575	-3.70278500	4.57626687
O	13.54411298	-0.77122127	0.47197448	H	26.6735906	-2.14077128	7.3425988	C	9.35901766	-2.30799617	4.90299835
H	10.81299576	-1.23900554	2.17599228	H	26.04125005	-2.06392949	8.37679991	H	8.53967094	-4.26584364	5.19629286
H	11.464305341	0.32122998	1.87482405	H	23.67452306	-1.81731502	7.32485846	H	10.25960733	-1.98190561	4.36692492
H	10.64400221	-0.40799862	0.61099924	C	24.47116607	-1.53356846	5.7917585	H	8.52599763	-1.68400312	4.58000133
N	12.53003395	-2.71604689	1.11744711	H	23.77409829	1.77863232	6.98632806	H	9.52299667	-2.18500116	5.97400145
C	13.72617679	-5.63736090	0.99601445	H	23.08679214	0.42365751	6.11161955	C	18.97699239	2.19998616	13.59598897
C	13.38951025	-4.78196142	0.16581699	H	26.19366442	-4.47161666	7.69273667	C	19.11567064	0.93587046	12.74963791
O	12.68078957	-5.695894192	0.619594917	H	24.50300074	-3.96499424	7.89300046	O	19.55623234	-1.1806441	13.20017307
C	14.27646101	-3.96102129	2.36633876	C	23.10292771	-2.60205388	3.93894329	H	18.10700229	-2.75800720	13.24900893
C	14.83324422	-2.80878098	3.21915833	C	21.69259647	-6.0544672	4.07086651	H	18.79700635	1.84600613	14.61100406
C	13.86789755	-2.21098123	4.23474712	C	21.56848678	-4.54536037	4.36302197	H	19.88548230	2.81806257	13.55396171
O	12.66249596	-2.10240554	4.04945355	O	20.61141188	-3.9244023	3.85338255	N	18.70060033	1.04801593	14.5111912
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H	14.48497087	-4.93511204	0.4789239	H	21.30700226	-6.47523724	5.15362986	O	20.40897947	-1.81965626	10.14865072
H	15.09715788	-4.67040443	2.17810070	H	20.98408930	-2.39494203	3.42194108	C	18.18591109	0.34123936	9.18432233
H	13.49117875	-4.97408975	2.91749320	H	22.37998210	-2.89458358	5.25935931	S	18.07196562	-1.06042749	7.98191949
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H	15.71928866	-5.623764357	3.76354919	H	23.39405775	-6.55396236	2.89001751	H	18.16960592	-0.93846262	10.96638551
H	13.8439770	-1.51940726	6.15097319	H	23.20701333	-7.62298655	4.030503608	H	18.84141480	1.11968960	8.77378488
H	15.37684203	-2.13197517	5.64193617	C	19.07994562	-5.21994884	8.05196552	H	17.18199538	0.76718283	9.32580094
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C	13.70800389	-5.95800437	-1.97500691	C	18.06728568	-3.99134254	1.12750245	C	22.50101362	0.02700000	9.97900474
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N	20.44553207	5.39758833	6.006741313	H	19.51209716	-5.57920088	1.25379328	C	25.3980028	-3.82699828	7.28700155
C	20.73356293	-7.01564494	5.55218479	H	17.47163091	-3.10829355	2.88589359	C	25.78146059	-2.34399057	7.34627162
O	21.90298549	-0.96708805	5.42471949	H	18.79533366	-3.96093743	2.98011134	C	24.63235013	-1.45781897	6.87191422
N	19.70490940	-3.77744745	5.15361376	H	18.93902598	-4.37401296	-1.52502116	C	24.74530756	0.00860105	7.28304536
C	18.38521839	-1.35947948	5.38686130	H	19.94581777	-5.80461425	1.20015334	O	25.52678346	0.40328421	8.14819212
O	17.49298041	-2.11378044	5.01507195	C	11.32700827	-0.6329952	1.43000245	N	23.88572490	0.83696797	6.63024501
N	16.87085810	0.49629325	5.70870802	C	12.56217920	-6.13649495	0.91577013	H	25.19600179	-4.16200130	6.27000045
C	16.51494518	1.71842745	6.26518367	O	13.43364729	-0.79752804	2.05169061	H	26.68497005	-2.14436426	6.74450425
C	15.18131061	2.11979857	4.61900217	H	10.81300015	-2.12390015	2.75998863	H	26.0356202	-2.06530744	8.83147133
C	14.84696124	3.36421121	6.95540347	H	11.65451416	0.3208803	1.86871852	H	23.67804929	-1.81540570	7.30146740
C	13.40262406	3.76693050	7.10748361	H	10.64399972	-6.05400216	0.61099943	H	24.47971144	-1.52299004	5.78087505
C	15.88427427	4.23994702	7.36079976	H	12.62852733	-2.68238791	1.26972227	H	23.80022351	1.78728126	6.97270878
C	15.56701084	5.59170867	7.951144608	C	13.79735129	-3.50897892	1.00076558	H	23.13236552	0.44155020	6.06646211
C	17.21633623	8.39548787	2.70012604	C	13.38964503	-4.73212034	0.15574659	H	26.19254283	-4.47370796	7.69280826
C	17.54878009	2.85961459	6.558570208	O	12.62446394	-5.12400598	0.60986434	H	24.50300074	-3.96500028	7.89299566
N	18.89190301	2.17472676	6.45747785	C	14.45878290	-3.99461759	3.20156283	C	23.10294067	-6.60200150	3.93985629
C	19.99614067	3.16222565	6.51351570	C	14.93751770	-2.87288550	3.23181680	C	21.69884944	-6.04274978	4.20932117
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C	18.05276099	-0.11167417	6.21214354	O	12.84570215	-3.03163410	3.47034693	H	22.50612623	-3.88130263	5.05701937
C	19.193494352	-2.45584714	4.67032125	H	11.47125105	-3.09743190	1.810448874	H	23.86761582	-6.03019600	4.49193720
H	14.39424079	1.40357167	6.10223121	H	11.86802094	-3.09743190	1.810448874	H	21.32538587	-6.43171864	5.17396686
H	13.15116512	3.96947917	8.16231416	H	14.51219148	-2.88481278	0.44944342	H	20.27998935	-6.36023803	3.44206953
H	13.18737137	4.69413008	6.55031631	H	13.76402005	-6.45287078	2.83821888	H	22.42108414	-2.86403374	5.17898807
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H	15.01182815	6.22195712	7.23648189	H	13.41940099	-0.87766595	5.40429155	H	23.20701666	-7.62298856	4.30502831
H	14.93187302	5.50373767	8.84889534	N	13.90638805	-4.80795348	-1.08907317	C	19.07993837	-5.21994238	-0.85196706
H	18.00457114	4.52598546	7.50490330	C	13.70800436	-5.95800036	1.97498521	C	19.27647528	-4.74448114	0.58144694
H	19.57629589	4.12440355	6.19726313	H	14.606009298	-4.11591383	1.345085873	C	18.02390770	-4.07474999	1.15117000
H	20.73692537	-3.70738872	4.59271243	H	12.91499940	-6.57700037	1.55700317	O	17.02161339	-3.84116230	0.46371541
H	21.29302663	4.21602017	8.101100046	H	13.43653342	-5.62247740	2.34781033	N	18.11492164	-3.78204133	2.46459129
H	16.11114346	-4.27723697	3.43315891	C	17.53447997	-2.55002198	1.62493868	C	11.32700231	-6.63031704	1.42997110
H	10.63363102	-6.06109811	1.76652408	C	15.61507991	-1.67127902	6.1983149	C			

C	20.62399350	3.25399923	7.90796057	C	13.79224361	-2.39732905	4.27772698	H	42.73884293	-26.78030149	4.39155768	
C	18.13098529	-0.22081619	6.20499447	O	14.19296034	-1.28460133	4.98743917	C	38.93604091	-23.77993020	5.17491983	
C	19.23365351	0.81473221	6.20512575	N	12.75129566	-3.09298884	4.50016548	C	38.52914171	-25.09944065	4.50382896	
H	20.12854876	-2.43469244	4.55462793	H	11.84563071	-3.10674593	1.77307014	C	39.03760235	-25.21827195	3.06017698	
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H	13.04705664	3.70085363	8.05571731	H	15.37839696	-4.46599208	2.05539163	O	39.46120610	-27.57837899	3.45436325	
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H	20.69547407	2.48833242	5.76187345	H	12.91500463	-5.67598672	-1.55697417	H	39.73414815	-26.02565404	0.69046520	
H	21.29300753	2.41601117	8.10102761	H	13.43699386	-5.62313635	-2.98726450	H	38.70101076	-23.78497855	6.25131859	
H	16.19058953	-0.33929873	5.44307670	H	14.62799314	-6.54203133	-2.01398764	H	40.01501594	-23.68606151	5.05604626	
H	21.20717392	1.48631018	7.95334715	N	20.49268695	0.53537311	5.98976458	C	38.54901538	-19.54504935	2.58497645	
H	19.84000740	3.28298023	8.66500762	C	20.80626707	-0.70369061	5.51206305	C	39.81670446	-19.64074745	1.73235270	
O	17.80957663	3.46336954	10.18793932	O	21.98427437	-1.05530689	5.36241755	C	40.05857371	-20.91598672	0.93708050	
H	17.75075360	4.38643851	10.47669113	N	19.79700238	-1.58535252	5.11240624	O	40.97206360	-20.95067303	0.08815869	
H	17.16131534	3.39679607	9.46409877	O	18.47108872	-1.39819685	5.35272307	N	39.31261614	-22.00325410	1.19378376	
AsLOV2 QdS <sub>0</sub>	C	5.51899781	-6.15600054	1.91000413	O	17.59205266	-2.14486468	4.95047745	H	38.38773761	-20.47590510	3.15873895
C	6.63784039	-5.97193288	2.92937738	C	16.90933479	0.38489237	5.74145668	H	40.71552994	-19.54047244	2.36903396	
O	6.42588167	-5.91704965	4.13988949	C	15.0953528	-0.70369061	5.51206305	H	39.88214538	-18.81172621	1.00970989	
H	5.84885209	-6.71110712	1.01891241	C	14.86221828	3.24640132	8.619612422	H	38.59173044	-21.99308506	1.90164956	
H	5.18999886	-5.16600225	1.59399700	C	13.37340892	6.32638740	7.00041153	H	38.44302091	-18.77600939	3.35200556	
H	4.68500049	-6.67600090	2.38199931	C	15.84119146	4.14039102	7.31126147	H	37.65100655	-19.36598720	1.99400577	
N	7.89688224	-5.87645625	2.406632860	C	15.49163285	5.49410473	7.87933266	C	39.25935451	-18.03510864	-3.47804361	
C	9.07818107	-5.74494449	3.25185763	C	17.18206824	3.75908694	7.17948321	C	40.08733417	-18.92764137	2.57288481	
C	9.46520581	-4.26102422	3.41001033	C	17.54617532	2.50922941	6.65845201	C	41.50871300	-19.17421865	3.08610876	
O	10.04205261	-6.44299449	2.50768842	N	18.90228425	2.17273263	6.47010767	O	41.87311932	-18.87336646	-4.22674036	
C	10.25301859	-6.53539004	2.68299202	C	19.98370929	3.14357422	5.16180692	N	42.31912054	-19.74280172	-2.16158600	
C	11.33924137	-6.73619693	7.34181660	C	20.62399889	2.35397402	7.90799581	H	39.81242479	-17.11220759	-3.70622996	
O	11.07208576	-6.81294065	4.94033207	C	18.12151206	-0.18027600	6.21785829	H	39.61484393	-19.1548872	-2.42677493	
N	12.58939685	-6.88297982	3.23084086	C	19.23437230	6.48251332	6.20488196	H	40.16431412	-18.49028574	-1.56203260	
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H	8.81358811	-5.73449449	2.42187497	H	14.42246610	3.20113157	6.03760528	H	41.93482210	-20.05339379	-1.27034977	
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H	38.95068896	-25.94212005	-5.09273018	H	50.13674537	-25.40437229	-6.31415635	O	40.17181573	-24.39438685	-0.09773014
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H	49.59528401	-21.40066097	-2.72138897	H	41.58532770	-22.48659867	-0.50686723	H	41.91557235	-20.08176020	-1.30954233
N	52.69668349	-22.27044644	-4.37205877	H	47.34708870	-25.19895773	-3.23542757	H	38.32705362	-17.73292112	-2.98896022
C	53.08493856	-26.56491174	-4.93901261	H	48.82789097	-27.45465531	-4.91864388	H	39.02799443	-18.49497510	-4.44001080
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H	52.98898814	-27.35597708	-4.19497610	H	47.47908218	-29.16961972	-4.68665298	C	47.52200528	-20.03571218	-9.36643974
C	47.64296096	-29.19898291	3.41493488	H	47.99428057	-29.09966050	-3.05348289	O	47.55708872	-18.62723734	-9.47553926
C	46.96639922	-28.35403425	3.38126054	H	44.66026888	-29.34624749	-2.72017602	H	48.03603948	-20.16305884	-7.28501237
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H	46.90198200	-30.49298911	3.57096611	H	42.48389660	-29.44230982	-0.34693501	H	47.18792938	-21.59500120	-7.90302027
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C	46.09097188	-26.58472636	1.88303528	O	46.74532484	-29.35989413	-0.21639355	C	44.84739847	-18.51908682	-5.73963843
C	44.54262465	-26.69240647	1.94901738	H	46.22401916	-30.35613049	-0.2380187	C	44.51645519	-17.11603984	-6.29520209
O	43.82397252	-26.15401725	1.09606060	H	46.48277397	-29.07159491	-0.12826662	O	45.38779189	-16.26336569	-6.46478351
C	46.52546540	-20.01733854	0.53385866	H	47.43473929	-22.30518466	-4.00938237	C	45.14421737	-18.44567017	-4.23201780
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H	46.83077316	-28.49544438	3.13156153	C	50.59295590	-14.38706594	-8.87698005	C	46.64311711	-20.57116086	-3.83074350
H	46.39023585	-25.90483557	2.69724446	C	50.85118984	-15.32366938	-7.70658687	O	46.76814333	-20.01929350	-4.25169015
H	45.96555878	-20.05886867	0.32002009	O	51.94899419	-15.79479950	-7.43320899	N	46.58259331	-21.87987510	-3.52328537
H	46.28116321	-26.72293539	-0.26359865	H	49.93901215	-13.56904074	-8.50998515	H	46.89151302	-18.98288171	-5.97460847
H	48.7845726	-26.75676754	0.83634283	H	50.09093270	-14.91296377	-9.69404306	H	43.98888202	-19.18600332	-5.90750700
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H	38.44596764	-23.20989976	4.74004834	C	50.46289418	-20.25355979	-5.87867369	N	41.79494164	-25.70087637	-1.09479780
H	37.43097281	-25.24033902	4.54466487	H	51.17226618	-21.05637647	-4.79218718	C	41.34358906	-24.46160175	-0.78181050
H	38.95126269	-25.94125794	5.09167682	O	51.83352713	-20.55359017	-3.89142160	O	40.29121526	-24.39940504	-0.17914720
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H	39.66816293	-26.09091641	0.70429086	H	50.88121489	-20.49054812	-6.86025058	C	46.60012930	-28.72844985	-3.16053150
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O	41.80473681	-18.49382682	-4.31615515	H	50.30777091	-21.5712839	-2.923093916	C	47.44125791	-27.59518550	-3.29883791
N	42.29071383	-18.88709830	-2.29292222	C	49.48353019	-21.42842820	-2.72042408	C	45.95010338	-28.94167209	-0.35781443
H	39.58705773	-17.11381832	-3.70616681	H	46.97882134	-28.36343069	-3.41798094	O	43.95510730	-22.32220616	-1.98571363
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H	48.36303239	-29.77835810	4.24137102	H	42.54003336	-28.38679388	0.48599615	H	48.10254039	-18.23758794	-7.88335854
H	46.90196660	-30.49297160	3.57097551	H	42.74574050	-29.53753779	-0.35966293	H	47.18794444	-21.59499729	-7.90293264
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C	44.7031996	-26.31916209	2.56101731	H	47.24577359	-29.88900919	-0.56343893	C	44.52005746	-17.04513474	-6.23576009
O	44.28314264	-25.17077480	2.60812807	H	46.45750094	-28.6981695	-1.12471925	O	45.36962111	-16.15685432	-3.34742818
C	46.37918149	-24.89977579	0.65783122	H	48.88638266	-19.78778216	-3.59932506	C	45.27206887	-18.43884209	-4.25611590
S	48.13117333	-25.76109791	0.15235157	RsLOV Qe S				C	45.81498203	-19.80768705	-3.77573311
H	46.69688634	-20.40090733	1.33248940	C	50.59334675	-14.38680775	-8.87728216	C	47.31842735	-19.79703952	-3.95617721
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H	45.96696792	-28.48224382	0.64788282	O	51.89760461	-15.89702935	-7.48269045	N	48.10579737	-19.34122657	-3.02971020
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H	48.26065348	-27.05787316	-0.23535636	H	50.09874404	-14.91309522	9.69378281	H	44.02744463	-19.14623904	-5.89787317
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H	37.42411457	-25.23969305	4.57300673	C	50.84723504	-20.99932987	-4.74616560	C	41.44697225	-24.48728000	-0.55912978
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H	38.22999283	-24.90082757	2.34287231	H	49.67182574	-20.40701807	-6.42376893	C	43.42284083	-23.35765718	-1.54115402
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H	39.81463077	-25.99712117	0.73809163	N	50.87901652	-23.31109116	-5.07955935	C	43.91782221	-24.69572287	-1.87932666
H	38.70624532	-22.77550104	6.25310308	C	51.02654251	-23.49106830	-4.15364738	N	45.11929540	-24.81354121	-2.50025552
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C	38.54901067	-19.54500580	2.58507406	O	51.11618689	-24.89511902	-6.02787746	C	46.75169444	-26.26949531	-3.48101980
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C	40.06964171	-20.88316107	0.90826071	O	48.7765081	-24.15749726	-4.71509593	C	48.59715438	-27.66213627	-4.48391214
O	40.92359668	-20.88548476	0.00366658	C	49.95211261	-22.97843250	-2.68403036	C	46.51453588	-28.67844991	-3.44769547
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H	43.18860554	-20.30028000	2.75002346	H	51.64930380	-23.09365989	-3.30810843	N	45.26362955	-28.51752568	-2.82062500
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H	38.32701970	-17.73279409	-2.98898570	H	49.29235374	-24.59304226	-5.346366520	N	43.49823784	-27.06703348	-1.90046801
H	39.02799075	-18.49500378	-4.43996976	N	47.99515641	-23.41452680	-3.25929621	C	43.07747244	-25.79064298	-1.53366140
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C	45.90716042	-20.05157924	-7.33763725	C	46.24554842	-26.51757726	-3.21370402	C	42.94960202	-28.944220264	-0.35788047
O	44.85282010	-20.64476614	-7.53930638	C	46.41147271	-25.18209264	2.54269668	O	46.88213338	-20.283781204	-3.27509581
C	47.44114874	-19.98486406	-0.35859771	H	46.69334212	-28.41854630	1.32367068	H	44.68129026	-29.41073565	-2.60906010
O	47.40709709	-18.57110227	-0.43343388	H	46.75874293	-25.28863658	2.79982022	H	42.72219676	-28.89355744	-2.52277376
H	48.03608288	-21.26106205	-7.28519488	C	45.95160968	-24.90481021	6.11359890	H	41.59845622	-27.84417414	-1.64213823
H	46.62638120	-20.35412187	-17.60607110	H	44.56414735	-28.28930545	2.80544381	N	42.54003585	-28.38691812	0.48596099
H	48.39263780	-23.30983636	-9.75747003	H	42.03327619	-26.87744258	2.75872874	C	42.47834422	-29.39358784	-0.35067929
H	48.07752507	-21.83758514	-8.81391069	N	47.90522774	-22.77721853	2.18108475	H	42.62229727	-27.52795274	-3.78990791
C	45.38462127	-17.19155787	-6.47331009	H	42.73867220	-26.77073002	1.34292906	C			

C	47.64288407	-29.70896746	3.41489092	H	48.06565103	-30.21418690	-3.23432496	O	47.47189743	-18.59409095	-9.44659930	
C	47.04265102	-28.33046655	3.46459590	H	44.71408501	-29.37136211	-2.63703518	H	48.03601339	-20.16300005	-7.28501380	
O	46.88842522	-27.67511296	4.47590745	H	42.76530548	-28.87303886	-2.53221030	H	46.67909386	-20.37036433	-10.02126425	
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H	48.36416859	-29.78577685	4.23977470	H	42.53995928	-28.38704956	0.48601028	H	48.08690194	-18.26509812	-8.76549389	
H	46.90198988	-30.49299716	3.57906176	H	42.47477951	-29.93686875	-0.36183513	H	47.18788255	-21.5949766	-7.90320594	
N	46.64449388	-27.80557494	2.22146076	H	44.02100426	-29.08501298	-0.21601225	N	46.00391169	-19.03042294	-6.46719401	
C	46.26823382	-26.45581476	2.12311513	O	46.96882217	-28.96610346	-0.27269184	C	44.88396366	-18.48052253	-5.73344208	
C	44.70730302	-26.30852579	2.58589538	H	47.40070806	-29.79250405	-0.53156851	C	44.53311438	-17.08121040	-6.27548447	
O	44.27928689	-25.16310310	2.63517886	H	46.51027071	-28.67982693	-1.09480143	O	45.39543247	-16.21498756	-6.42459683	
C	46.4292704	-25.83306013	0.73033779	H	47.32839731	-22.55855915	-4.22411015	C	45.21410650	-18.40597426	-4.23279004	
S	48.18420954	-25.67990872	2.59889899	RsLOV Qa T <sub>i</sub>	C	50.59293314	-14.38705260	-8.87679418	C	45.3910268	-19.78082607	-3.585939491
H	46.73453831	-28.35296801	1.34740653	C	50.86129999	-15.33268404	-7.71134762	C	46.69440069	-20.53558523	-3.89146080	
H	46.76382620	-25.86990177	2.9102607	O	51.94271561	-15.86569602	-7.49805744	O	47.73919581	-19.96925021	-4.24778431	
H	46.00645275	-24.81732727	0.73811534	H	49.93902294	-13.55909593	-8.50989716	N	46.60789185	-21.87096841	-3.7068207	
H	45.87450748	-26.40173946	-0.28406663	H	50.09903900	-14.91297774	-9.69403851	H	46.93310180	-18.72532961	-6.20399157	
H	48.31046223	-26.95725271	-0.18661622	H	51.54377486	-13.97326716	-9.23464493	H	44.03340066	-19.15980344	-5.88603531	
N	44.05972543	-27.40813769	1.392189358	N	49.79232474	-15.49848381	-8.61615977	H	44.37314278	-17.90253513	-3.73207827	
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C	38.93603588	-22.39972723	5.17489052	H	50.77941679	-15.2028167	-5.21096942	N	43.21297341	-16.89973144	-6.5631866	
C	38.51873967	-25.40439049	5.07808951	H	48.01309466	-15.5374169	-3.90973185	C	42.65097664	-15.60801734	-6.94400515	
C	38.99563558	-25.22201546	3.06109640	H	48.60134684	-17.13840969	-4.13478922	H	42.57489450	-17.62324972	-6.24176726	
C	39.46443848	-26.63326101	2.67719723	H	48.62481103	-15.35657994	-3.40685248	H	43.45498289	-14.86185546	-6.86843023	
O	39.63446772	-27.52878794	3.50888559	H	47.69219799	-16.39286244	-5.47474156	C	42.26011163	-15.58400021	-7.96200211	
N	39.71674013	-26.795694032	1.35559886	N	50.59864905	-17.89096296	-5.59773643	H	41.86001514	-15.35199303	-6.23899045	
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H	37.42521695	-23.23949848	4.56883991	C	51.17432161	-21.02453855	-4.80935153	C	41.34352423	-24.46193133	-6.99314269	
H	38.95847914	-25.94043904	5.07808951	O	51.84764669	-15.5374169	-3.90973185	O	40.26542729	-24.37974970	-0.07826451	
N	39.85933456	-25.55270701	2.87279740	H	51.10096029	-18.53577027	-4.75245006	N	42.08126884	-23.34498907	-0.99084544	
H	38.22850029	-22.89552623	3.33929313	H	49.39416633	-20.47624848	-5.82997179	C	43.32779106	-23.35603287	-1.62176124	
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H	39.83115005	-25.98038021	4.73243616	N	50.97383334	-22.36587460	-4.97091676	C	43.84488894	-24.69096297	-1.92739106	
H	38.70547209	-23.77787794	6.25279409	C	51.24555787	-23.33670743	-3.91939324	N	45.09434014	-24.79441786	-2.45493335	
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C	40.09339865	-20.89155522	0.93909040	O	48.86125526	-23.81489717	-3.80241360	C	48.79314597	-27.66720872	-3.86200289	
O	40.99720672	-20.88402358	0.80369542	C	49.68506708	-22.31230366	-2.14167364	C	46.53258199	-28.67286883	-3.28313755	
N	39.39368832	-22.00420259	1.20858931	H	50.25074729	-22.65097197	-5.62511405	C	47.06914338	-30.04369789	-3.60077594	
H	38.39317226	-20.48002225	3.15305391	H	52.09632327	-22.96505583	-3.33106995	C	45.22933744	-28.51159138	-2.82191659	
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H	39.81410107	-17.11352376	3.70858588	H	47.63455538	-29.06846460	-3.41558105	C	47.40603518	-30.10993369	-6.464848975	
H	39.58222750	-19.89833422	2.38867575	C	46.96061878	-28.35675570	-3.36024093	C	47.94165305	-30.28921121	-2.97206711	
H	40.25742830	-18.48385682	1.60146456	O	46.61931800	-27.73439441	-3.465945303	H	44.60904386	-29.39858950	-2.70499533	
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H	41.93936829	-20.18434455	-1.40170666	H	48.34927516	-27.20870583	-4.25628760	H	41.55767570	-27.89615718	-1.64754846	
H	38.32704103	-17.73294250	2.98863973	H	46.90138442	-30.49591460	-3.15088217	H	42.53981397	-28.38713254	0.485939431	
H	39.02797260	-18.49501304	-4.03988636	H	46.37170027	-27.8957226	-2.09835303	C	42.48163722	-29.94073434	-0.35506328	
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C	45.87800291	-19.9666937	1.749081136	C	44.52202605	-26.73004399	1.90390673	O	46.72497703	-29.62250503	-0.20419432	
O	44.82280569	-20.34174549	17.99757700	H	43.79170487	-26.16925188	1.04668341	H	46.20678174	-30.43990967	-0.24377857	
C	47.55096868	-20.20363733	9.36262484	C	46.48646684	-26.11033054	0.44367147	H	46.52545170	-29.17530506	-1.04544317	
O	40.3600112	-20.16299936	-7.28499760	H	46.80339887	-23.56125408	1.31588217	C	50.59308571	-14.38695904	-8.87703704	
H	46.72931379	-20.14394316	-10.03194194	H	46.383238							

S	48.25909859	-25.73554070	0.24442173	RsLOV	Qc	T <sub>1</sub>	C	45.82274410	-19.80057671	-3.77908067
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H	46.39171284	-25.92799598	2.58253071	C	50.84302803	-15.32871113	-7.70542755	C	47.82397757	-20.67374866
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H	48.71325814	-26.91970916	0.73159045	H	50.09876658	-14.91310210	-9.63979170	H	44.07895790	-19.13946531
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H	42.73900269	-26.78098121	4.39198794	C	48.58239573	-18.20229519	-4.85364770	H	47.72209053	-18.95891226
C	38.93603557	-27.77995168	5.17491187	H	48.85344058	-15.19216822	-7.19135699	N	43.21353693	-16.89153544
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C	39.04264446	-25.25981115	3.08546162	H	48.56699159	-16.95946714	-4.05638188	H	42.58134369	-17.16182323
C	39.36370958	-26.72141191	2.70361479	H	48.00660871	-15.20014614	-4.39781405	H	43.45089732	-14.85782419
O	39.46140888	-27.61060084	3.53623781	H	47.64632245	-16.29540933	-5.43019653	H	42.26205801	-15.58397311
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H	39.98936505	-27.40183576	2.95602968	H	50.99305877	-18.46561580	-4.70584603	N	42.04620261	-23.37348910
H	38.34950958	-24.83240977	2.34114376	H	49.66367906	-20.43315932	-6.40624719	C	43.1047617	-23.36598293
H	39.92895507	-27.82493265	1.10542727	H	51.42100859	-20.28320282	-6.67530530	O	43.91079368	-22.31074747
H	39.68682161	-26.13405063	0.72796636	N	50.86923691	-20.32728213	-5.03672130	C	43.81193559	-24.69276169
H	38.70430763	-23.77256694	6.25229524	C	51.04749233	-23.41392502	-4.08873096	N	45.04364829	-24.78702726
H	40.01501221	-23.68603574	5.056036379	C	51.59165582	-16.46095494	-4.87959460	C	45.44010625	-26.03621567
C	38.54901554	-19.54503924	2.58504021	O	50.99226405	-24.95930044	-5.90803760	C	46.71010515	-26.21317969
C	39.81497802	-19.64804428	1.72922344	C	49.69712946	-23.89677973	-3.47414134	C	47.2308121	-27.46399553
C	40.02899439	-20.92334494	0.92058581	O	48.76024797	-24.14558755	-5.41333933	C	48.59957595	-27.59353383
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H	40.71401365	-19.56868949	3.26642914	H	49.9225679	-24.84123877	-2.92318608	C	44.65301055	-27.23291642
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H	39.53375265	-22.90719078	0.75712123	H	48.13377736	-23.35344713	-2.11375805	C	42.96093747	-25.79807374
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H	37.65101053	-19.36598990	1.99390964	N	52.6376255	-25.29411142	-4.37081719	H	41.65191407	-22.46245586
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O	41.83395459	-18.81558200	3.42711076	H	54.12656418	-26.50360947	-5.28932018	H	49.27831239	-28.13630480
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C	47.23005512	-20.50604010	7.93404514	C	46.06091900	-26.64207848	1.79223826	H	44.020101215	-29.08499408
C	45.91186914	-20.06049286	-2.73207554	C	44.51403379	-26.72836126	1.89705884	O	46.73850137	-29.58710995
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C	47.43270148	-19.97494309	-3.93558626	C	46.46386293	-26.14014194	0.40612326	H	46.54227710	-29.11747099
O	47.39735589	-18.56026213	-9.42009292	S	48.24582953	-26.72985400	0.22514275	C	50.59299966	-14.38701905
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H	48.08668921	-18.23260666	-8.81516103	H	46.17788321	-26.87958735	-0.35498637	H	49.33809760	-13.59600797
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H	37.43073770	-25.23940560	4.54206358	C	51.06806705	-21.03161122	-4.72706075	O	40.16828009	-24.25844359	-0.11728564
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C	45.85540386	-20.0741442	-7.50891695	C	46.07457807	-26.61485983	1.84100480	O	46.75614017	-29.55265294	-0.25441541
O	44.82509788	-20.3699893	-8.07163308	C	44.52818663	-26.70426178	1.92982789	H	46.19483006	-30.34194558	-0.27356316
C	47.56581142	-20.00621166	-9.34807126	O	43.80936285	-26.15483493	1.09703751	H	46.54137983	-29.09603383	-1.08731942
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C	47.89402847	-21.36001052	-6.71904746	N	47.11887471	-28.55907376	3.48801499	H	44.3789521	-29.74502914	0.91601107
C	46.57334076	-20.79915138	-6.20624015	C	46.65289832	-27.19331777	3.26796652	H	42.72050921	-30.40859550	0.77636349
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O	48.18927355	-19.44975643	-8.23675966	C	46.42761137	-26.99598831	1.75059397	H	46.98969604	-29.58725426	0.16979537
H	48.69009948	-21.07099254	-6.03301144	S	46.00803499	-25.23960420	1.35486795	RsLOV Qd <sub>S<sub>0</sub></sub>			
H	47.42552039	-21.23135314	-8.82385034	H	47.22047759	-29.18017609	2.68459977	C	51.38378071	-15.19413511	-7.59191856
H	49.17311688	-21.29318681	-8.46669247	H	47.39351279	-26.47374461	3.65124242	C	51.64681996	-16.18914630	-6.47026483
H	48.76159002	-21.15030924	-7.52981805	H	45.60788465	-27.65185784	4.14065553	O	52.73124495	-16.72141141	-6.26419522
H	47.77599945	-22.44400664	-6.70596249	H	47.33654738	-27.27455192	1.19703087	H	50.77610663	-14.39091306	-7.17601953
N	46.72197352	-19.77959059	-5.29513478	N	44.48528263	-27.93051024	4.07965019	H	52.33644920	-14.81057072	-7.97512856
C	45.60474250	-19.15157479	-6.63798074	C	43.17402000	-25.76679499	4.66404033	H	50.83307267	-15.68294614	-8.39508061
C	45.38795059	-17.75520864	-5.23867958	H	44.82384251	-28.84585307	3.81459017	C	50.56679756	-16.42374534	-5.65520449
O	46.32631230	-16.97083556	-5.39699949	H	42.52495245	-27.18888866	3.99314274	O	50.64986992	-17.42089911	-6.40305745
C	45.84528457	-19.04243404	-3.12332252	H	42.70598906	-28.75200099	4.80096534	C	50.86360505	-18.81436602	-5.20714528
C	46.02632716	-20.40857279	-2.44771769	H	43.21399711	-27.24410898	5.61401042	O	50.22486502	-19.21313467	-6.18444477
C	47.29242993	-21.16321305	-2.76994429	C	39.62405177	-24.39400617	6.51682846	C	49.38179835	-17.40388988	-3.74449309
O	48.38083767	-20.33485041	-2.75994463	C	39.19921666	-25.70189014	5.83754072	H	49.63835956	-16.15834279	-5.96723634
N	47.27569299	-22.42308047	-2.97293289	C	39.72803393	-25.83146953	4.40631951	H	51.53341092	-17.18066217	-3.99000056
H	47.64173676	-19.38596803	-5.17339802	C	39.84346183	-27.28414713	3.92806399	H	49.35997846	-18.27495320	-3.07343694
H	44.72516667	-17.78494884	-4.81687938	O	39.73733745	-28.23456604	4.68621214	H	49.34220800	-16.47913173	-3.14884983
H	44.96453026	-18.55397704	-2.68208355	H	40.09629812	-27.14211311	2.59471717	H	48.47445193	-17.43592902	-4.36859558
H	46.72144376	-18.40389779	-2.93505953	N	39.15996083	-23.50698967	6.08670045	N	51.77317230	-19.58710074	-4.57188959
H	45.19002830	-21.07388962	-2.69784780	H	38.10119686	-25.51847954	5.84371092	C	52.05444905	-20.94343664	-4.97029080
H	46.02103841	-20.25869031	-1.35403074	H	39.59039721	-26.55795966	6.41305066	C	52.16370273	-21.83950501	-3.73955359
H	48.20277223	-22.80145860	-3.19322126	C	40.74480723	-25.40238282	4.33127499	H	51.27831262	-19.23322782	-3.76736752
N	44.09934700	-21.46502541	-5.56044483	H	39.11850922	-25.26050968	3.68455085	O	52.60843165	-21.43435663	-2.67257269
C	43.67000613	-16.12803914	-5.96460403	H	40.35667297	-28.35057343	2.28417533	H	52.27831262	-19.23322782	-3.76736752
C	42.74755990	-26.29974187	0.63428192	H	40.44426555	-26.62297042	2.06002146	N	51.26205232	-21.26690173	-5.65934134
C	42.32789028	-25.06857022	1.05830217	H	39.36214703	-24.40095716	7.58764672	C	50.17440580	-23.20525122	-1.20310547
O	41.29881299	-24.95794397	1.73983674	H	40.70807921	-24.31400376	6.43607347	H	51.32747255	-23.37567937	-4.83137011
N	43.00443905	-23.91649483	0.66737230	C	39.31105726	-22.10020445	3.83696928	N	51.75957239	-23.12292253	-3.94955086
C	44.18612926	-23.90294163	-0.02436377	C	40.56902179	-20.08822649	2.96072477	C	51.82074978	-22.16575619	-2.93929252
O	44.71700125	-22.89089611	-0.44475643	C	40.86318967	-21.40203947	2.32994143	C	52.08238427	-25.48776653	-3.66588866
C	44.85722957	-27.25290767	-0.21062496	O	41.75346536	-21.4442252	1.36490773	H	51.27444441	-25.84967826	-4.53740839
N	45.46775752	-25.33237569	-0.46433796	H	39.39790093	-17.26500340	2.32841753	C	50.46396799	-24.32153073	-2.19119086
C	46.00371145	-26.56158020	-1.85401823	H	40.18467855	-22.50060774	2.59761398	O	49.40856556	-24.35988968	-3.16611095
C	47.14754136	-26.68560416	-2.65496395	H	39.36214703	-24.40095716	7.58764672	C	50.17440580	-23.20525122	-1.20310547
C	47.66879698	-23.93690186	-2.99788500	C	40.95800384	-23.34120026	-1.30603517	H	51.32747255	-23.37567937	-4.83137011
C	48.91111386	-28.03494428	-3.84864429	C	42.31054295	-19.72776204	-1.91402253	C	53.45893776	-27.54097399	-3.80009271
C	47.02557960	-29.10792894	-2.53240775	O	42.63556774	-19.43645535	-0.06771134	C	53.75459226	-25.82118587	-2.56897124
C	47.56203965	-20.30745130	-2.88138337	H	43.11534636	-20.40837333	-0.10755553	H	52.79002379	-27.74801898	-4.63601233
C	45.87131543	-28.98261051	-1.74922628	H	40.65949093	-17.55231510	-2.48333789	C	50.46396799	-24.32153073	-2.19119086
C	43.18263711	-28.70221796	-0.51875257	H	41.15215405	-18.83489359	-0.34370794	C	49.40856556	-24.35988968	-3.16611095
C	43.32601911	-29.48993311	0.79379306	H	43.92334550	-20.90264044	-1.41994616	H	50.17440580	-23.20525122	-1.20310547
C	42.55481603	-23.00706038	0.90297497	H	42.76305993	-20.83320708	-1.81301585	N	51.32747255	-23.37567937	-4.83137011
H	45.95279761	-24.47920338	-1.78918128	H	43.17997284	-18.16305232	-1.73302163	C	52.60775292	-23.89882622	-2.21976335
H	47.63773719	-23.77300734	-3.00939258	H	39.88193286	-18.96899038	-3.15999023	C	52.079002379	-27.74801898	-4.63601233
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H	49.28953465	-27.04640446	-4.12997520	H	46.59673060	-22.85512997	-6.09893962	C	50.90446328	-23.23240860	-0.38092157
H	49.71930135	-28.57033238	-3.32063860	H	45.54902278	-21.49667721	-6.14213810	C	50.23538602	-22.21647252	-1.67616991
H	46.94926526	-31.27585198	-2.44193798	C	48.16527568	-28.83320786	-8.13105185	H	53.14857847	-26.21156856	-3.28136529
H	47.58095160	-30.63355267	-3.97278309	H	48.21255878	-19.42070502	-8.20616474	C	53.45893776	-27.54097399	-3.80009271
H	48.59948763	-30.60825556	-2.52299907	H	48.69000044	-16.08709558	-6.03030454	C	53.75459226	-25.82118587	-2.56897124
H	45.36417016	-29.88739306	-1.41414557	H	47.35228656	-21.15483936	-8.80461458	H	52.79002379	-27.74801898	-4.63601233
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H	42.18508820	-28.25285789	-0.59612874	H	48.83547679	-19.11463117	-5.72395154	C	53.70993676	-25.85155484	3.4930921
H	43.00399600	-28.86004110	-1.62027126	H	47.77600141	-22.44400446	-6.70601250	C	39.19953991	-25.70171374	5.83703032
H	44.37899818	-27.45015152	0.91610107	H	46.71556004	-19.66891109	-5.43308647	C	39.72499730	-25.82880044	4.40430506
H	42.71643174	-20.40502878	0.76130691	C	45.64556224	-19.13311968	-4.61296689	H	40.85399859	-20.55520993	6.41048172
H	46.92742458	-20.05406311	0.98232627	C	45.37646400	-17.69268624	-5.07188055	C	43.17401808	-27.77697201	4.66402666
H	47.00039457	-30.97743157	0.71219850	H	46.27414045	-16.84607112	-5.04524				

H	48.68980151	-21.07129253	-6.03268642	C	43.66996517	-16.12801516	-5.96408642	C	45.84042328	-29.06653569	-1.63491497
H	47.44405181	-21.17570094	-8.82915915	H	43.40797137	-18.17696143	-5.39768626	C	43.14518073	-28.71909903	-0.51899420
H	49.18201885	-21.34993171	-8.46076500	H	44.54599620	-15.48499612	-5.87895841	C	43.32606409	-29.48986310	0.79397006
H	48.97608323	-19.17080620	-7.54823418	H	43.27301492	-16.11768181	-6.99066499	H	42.51578466	-22.98656496	0.78289677
H	47.77579244	-22.44397662	-6.70589550	H	42.90904210	-15.80299413	-5.25496238	H	46.06455752	-24.57015185	-1.68562515
N	46.68883311	-19.70530660	-5.44339299	C	45.34413344	-27.79255034	-1.32619726	H	47.85448914	-25.93776817	-2.68336867
C	45.60416644	-19.17148832	-4.64225298	N	44.11660786	-27.60547144	-0.64218423	H	48.97776919	-28.82781188	-4.35989029
C	45.36002824	-17.71808971	-5.08300631	C	43.81009834	-26.41178467	-0.07709801	H	49.55380186	-27.29039062	-3.69084639
O	46.25916235	-16.87654945	-5.03760860	N	42.66609952	-26.28481790	0.549161344	H	49.83244924	-28.81178834	-2.81435723
C	45.93768151	-19.27566225	-3.14317145	C	42.24736945	-25.04323055	0.94201768	H	46.86804623	-31.40183490	-2.24980357
C	46.09116482	-20.72730017	-2.66621906	O	41.19972725	-24.90860695	1.58815641	H	47.68069352	-30.78460494	-3.70334463
C	47.37071927	-21.46371233	-2.99419505	N	42.95184635	-23.90366904	0.5307121	H	48.54821977	-30.81113318	-2.16527995
O	47.19033058	-22.80771115	-2.86310794	C	44.15886896	-23.9204516	-0.09229051	H	45.27319798	-29.95082252	-1.34736439
N	48.46644289	-20.88280382	-3.31285218	O	44.71753805	-22.92735146	-0.52383679	H	43.28189711	-29.36258565	-1.39680463
H	47.62703045	-19.42602728	-5.18230268	C	44.83127586	-25.30143761	-0.19455962	H	42.14441807	-28.27618037	-0.57700458
H	44.71926947	-19.78667930	-4.85639456	N	45.53617520	-25.40579184	-1.42779380	H	43.00397311	-28.86006206	1.62303412
H	45.10273421	-18.82443921	-2.58689904	C	46.07527484	-26.65288439	-1.72104741	H	44.37899019	-29.74505317	0.91600407
H	46.84624979	-18.69572066	-2.92304601	C	47.28876543	-26.82640134	-2.40056789	H	42.72301354	-30.41056103	0.78447195
H	45.26018805	-21.34195357	-3.04744552	C	47.78928397	-28.09663058	-2.70303158	O	46.94546677	-30.09583148	1.05495449
H	46.00877748	-20.77088236	-1.56619854	C	49.10231465	-28.25377611	-3.42631065	H	47.01694189	-31.03075031	0.81369568
H	49.20395754	-21.57757640	-3.48065632	C	47.05280656	-29.23992491	-2.31343013	H	46.99176782	-29.62492956	0.20437986
N	44.11244937	-17.46774742	-5.56751644	C	47.55870647	-30.62874276	-2.61843703	H	48.02717370	-23.28739186	-3.06344025