

# Racemization of oxazepam and chiral 1,4-benzodiazepines. DFT study of the reaction mechanism in aqueous solution.

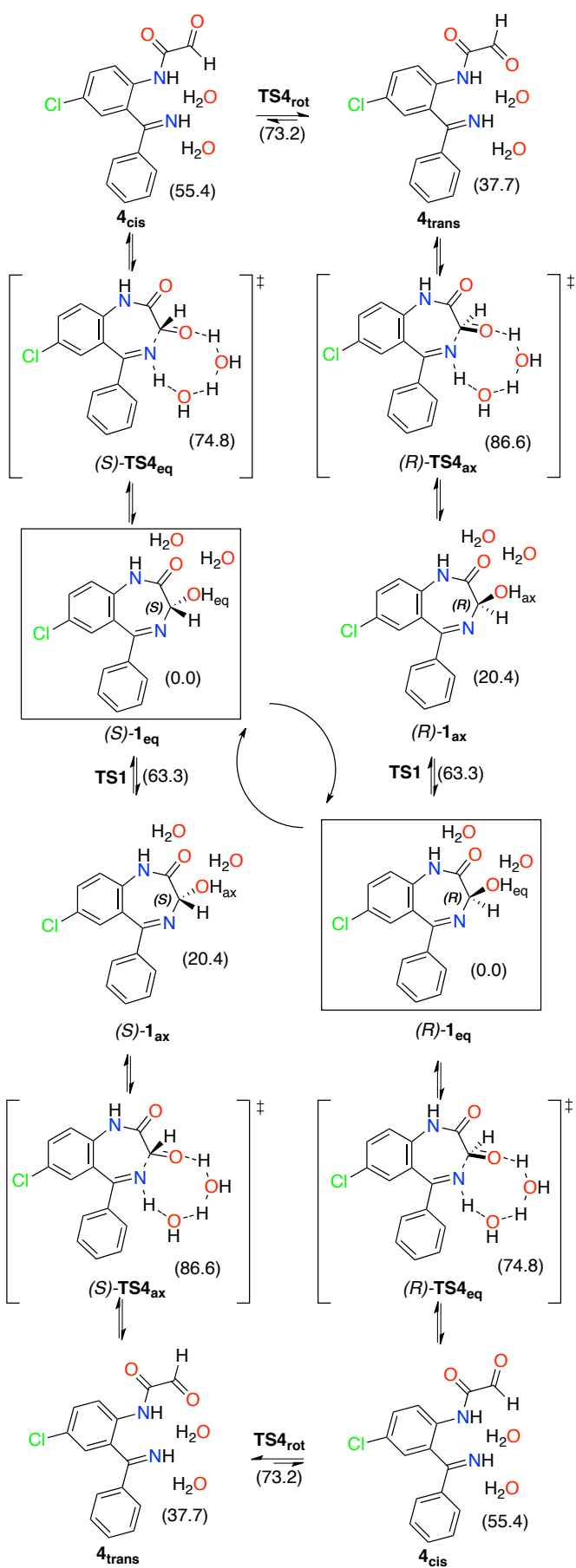
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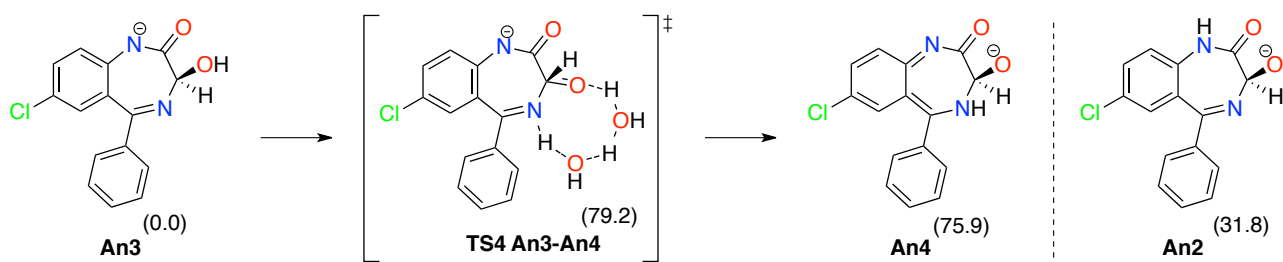
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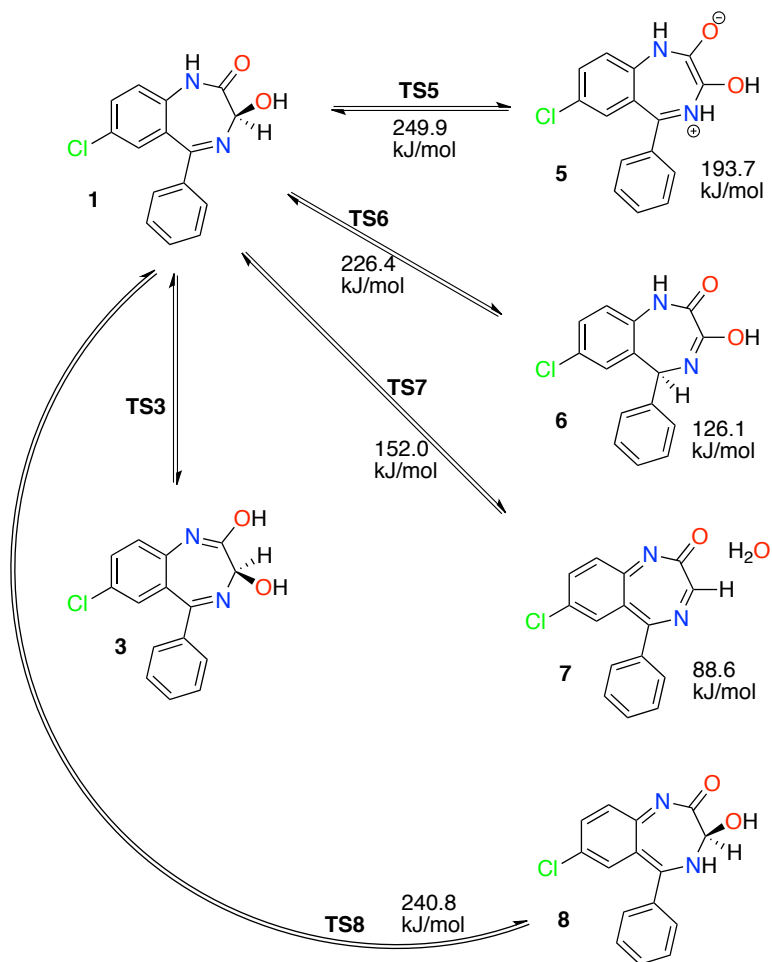
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**Scheme S1.** Full Mechanism IV scheme (for clarity purposes, only half is in the MS).

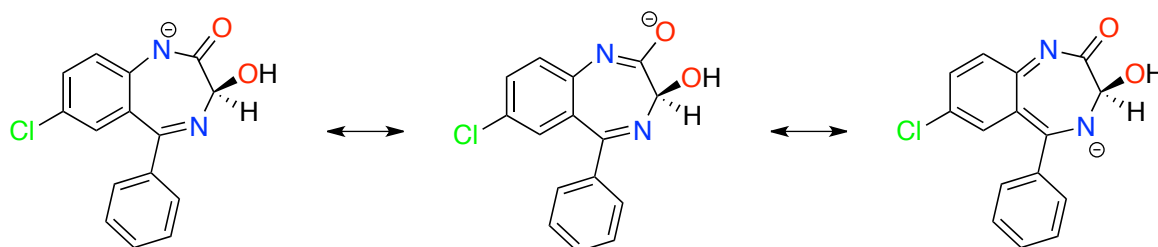


**Scheme S2.** Proton transfer mechanism from C3-OH to N4 in anionic form **An3**.

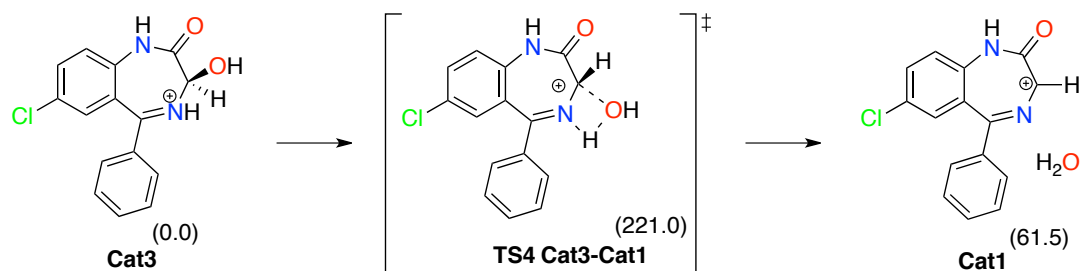


**Scheme S3.** Alternative mechanisms for racemization, not discussed in the manuscript.

The labeled numbers are calculated Gibbs free energies using two explicit water molecules on B3LYP/6-31+G(d) level of theory.



**Figure S1.** Resonance stabilisation of the N1-anion of oxazepam



**Scheme S4.** Proton transfer mechanism from N4-H to C3-OH in cationic form **Cat3**.

**Equation 1.** Calculation of relative  $\Delta pK_a$  values

$$\Delta pK_a = pK_{a1} - pK_{a2}$$

$$\Delta pK_a = -\log\left(\frac{K_{a1}}{K_{a2}}\right)$$

$$\Delta G_a = G_{an} + G_{H^+} - G_{neut}$$

$$K_{a1} = \exp\left(\frac{-\Delta G_{a1}}{RT}\right) \text{ and } K_{a2} = \exp\left(\frac{-\Delta G_{a2}}{RT}\right)$$

$$\Delta pK_a = -\log\left(\frac{\exp\left(\frac{-\Delta G_{a1}}{RT}\right)}{\exp\left(\frac{-\Delta G_{a2}}{RT}\right)}\right)$$

$$\Delta pK_a = -\log\left(\exp\frac{\Delta G_{a2} - \Delta G_{a1}}{RT}\right)$$

$$\Delta G_{rel.acid.} = \Delta G_{a2} - \Delta G_{a1}$$

$$\Delta pK_a = -\log\left(\exp\frac{\Delta G_{rel.acid.}}{RT}\right)$$

For change of one  $pK_a$  unit, corresponding  $\Delta G_{rel.acid.}$  equals to 5.7077 kJ/mol.

Due to large error of the  $G_{H^+}$  value, isodesmic reactions are used to evaluate  $\Delta pK_a$  values.

$$\Delta G_{rel.acid.} = G_{an2} - G_{an1} + G_{neut1} - G_{neut2}$$

Last equation is extensively used in this SI to calculate relative acidity of different benzodiazepines to N1-anion of oxazepam (OXZ **An3**).

Table S1. Energies of calculated stationary points for C3-OH configuration inversion in oxazepam (OXZ)

Inversion	B3LYP/6-31+G(d)				B2PLYP/aug-TZVPP		B3LYP/6-31+G(d)		B2PLYP/aug-TZVPP		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	SP(Hartree)	G(Hartree)	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
<b>1<sub>eq</sub></b>		-1298.402298	0.188485	-1298.213814	-17.14	-1297.910748	-1297.722264	0.00	0.00	0.00	0.00
<b>TS1</b>	<b>0<sub>w</sub></b>	-1298.375538	0.188167	-1298.187370	-17.27	-1297.882438	-1297.694270	69.43	68.88	73.50	72.95
<b>1<sub>ax</sub></b>		-1298.391198	0.188327	-1298.202871	-17.77	-1297.899340	-1297.711013	28.73	26.09	29.54	26.90
<b>1<sub>eq</sub></b>		-1374.825102	0.200606	-1374.624496	-26.99	-1374.324852	-1374.124246	0.00	0.00	0.00	0.00
<b>TS1</b>	<b>1<sub>w</sub></b>	-1374.808339	0.205810	-1374.602529	-23.58	-1374.305030	-1374.099220	57.67	71.94	65.70	79.97
<b>1<sub>ax</sub></b>		-1374.827437	0.205842	-1374.621595	-23.27	-1374.324875	-1374.119033	7.62	23.18	13.69	29.25
<b>1<sub>eq</sub></b>		-1451.283289	0.230495	-1451.052795	-21.43	-1450.770405	-1450.539911	0.00	0.00	0.00	0.00
<b>TS1</b>	<b>2<sub>w</sub></b>	-1451.242314	0.223427	-1451.018887	-27.89	-1450.728947	-1450.505520	89.03	62.00	90.29	63.26
<b>1<sub>ax</sub></b>		-1451.275928	0.231660	-1451.044268	-22.42	-1450.762207	-1450.530547	22.39	18.25	24.58	20.44
<b>1<sub>eq</sub></b>		-1527.718428	0.248700	-1527.469728	-26.02	-1527.194640	-1526.945940	0.00	0.00	0.00	0.00
<b>TS1</b>	<b>3<sub>w</sub></b>	-1527.680636	0.245033	-1527.435603	-30.04	-1527.157256	-1526.912223	89.60	72.78	88.53	71.71
<b>1<sub>ax</sub></b>		-1527.709240	0.248053	-1527.461187	-27.26	-1527.185354	-1526.937301	22.42	17.24	22.68	17.49
<b>1<sub>eq</sub></b>		-1604.151565	0.266790	-1603.884775	-31.64	-1603.617546	-1603.350756	0.00	0.00	0.00	0.00
<b>TS1</b>	<b>4<sub>w</sub></b>	-1604.115229	0.264138	-1603.851091	-34.71	-1603.581869	-1603.317731	88.44	75.59	86.71	73.86
<b>1<sub>ax</sub></b>		-1604.135753	0.262087	-1603.873666	-33.77	-1603.602092	-1603.340005	29.17	20.25	28.23	19.32

Table S2. Energies of calculated stationary points for Mech I of oxazepam (OXZ)

Mech I	B3LYP/6-31+G(d)				B2PLYP/aug-TZVPP		B3LYP/6-31+G(d)		B2PLYP/aug-TZVPP			
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	SP(Hartree)	G(Hartree)	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta pK_{\text{a}}$
<b>An1</b>		-1297.852649	0.174237	-1297.678412	-48.63	-1297.356148	-1297.181911	39.66	70.75	36.34	67.43	11.83
<b>An2</b>	<b>0<sub>w</sub></b>	-1297.822038	0.172320	-1297.649718	-75.21	-1297.318919	-1297.146599	115.00	34.87	148.49	68.37	11.99
<b>An3</b>		-1297.868704	0.175186	-1297.693518	-56.06	-1297.370940	-1297.195754	0.00	0.00	0.00	0.00	0.00
<b>An1</b>		-1374.293980	0.193690	-1374.100290	-50.42	-1373.787747	-1373.594057	38.20	69.95	32.51	64.27	11.27
<b>An2</b>	<b>1<sub>w</sub></b>	-1374.274469	0.191852	-1374.082617	-72.06	-1373.762044	-1373.570192	84.60	25.81	109.50	50.71	8.90
<b>An3</b>		-1374.308421	0.193582	-1374.114839	-58.01	-1373.800021	-1373.606439	0.00	0.00	0.00	0.00	0.00
<b>An1</b>		-1450.735483	0.214315	-1450.521168	-50.6	-1450.218451	-1450.004136	53.47	81.21	47.77	75.51	13.25
<b>An2</b>	<b>2<sub>w</sub></b>	-1450.725030	0.210926	-1450.514105	-72.42	-1450.201682	-1449.990757	72.01	8.46	95.38	31.83	5.58
<b>An3</b>		-1450.758886	0.217352	-1450.541534	-57.23	-1450.239684	-1450.022332	0.00	0.00	0.00	0.00	0.00
<b>TS</b>		-1450.715880	0.214719	-1450.501160	-65.52	-1450.193686	-1449.978966	106.00	71.32	113.86	79.17	
<b>An3-An4</b>	<b>2<sub>w</sub></b>	-1450.723416	0.218910	-1450.504505	-65.52	-1450.199122	-1449.980211	97.22	62.53	110.59	75.90	13.32
<b>An1</b>		-1527.173447	0.231783	-1526.941665	-54.05	-1526.645427	-1526.413645	63.25	80.78	57.20	74.73	13.11
<b>An2</b>	<b>3<sub>w</sub></b>	-1527.170271	0.231946	-1526.938325	-70.06	-1526.637221	-1526.405275	72.02	22.57	91.09	41.64	7.31
<b>An3</b>		-1527.200613	0.234855	-1526.965757	-58.24	-1526.670286	-1526.435430	0.00	0.00	0.00	0.00	0.00
<b>An1</b>		-1603.611804	0.248423	-1603.363381	-56.83	-1603.072454	-1602.824031	56.99	75.40	52.96	71.36	12.52
<b>An2</b>	<b>4<sub>w</sub></b>	-1603.616536	0.252379	-1603.364157	-72.3	-1603.072845	-1602.820466	54.96	8.64	71.70	25.38	4.45
<b>An3</b>		-1603.638371	0.253282	-1603.385089	-61.23	-1603.097482	-1602.844200	0.00	0.00	0.00	0.00	0.00

Table S3. Energies of calculated stationary points for Mech II of oxazepam (OXZ)

Mech II	B3LYP/6-31+G(d)				B2PLYP/aug-TZVPP		B3LYP/6-31+G(d)		B2PLYP/aug-TZVPP		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	SP(Hartree)	G(Hartree)	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
	1 <sub>eq</sub>	-1298.402298	0.188485	-1298.213814	-17.14	-1297.910748	-1297.722264	0.00	0.00	0.00	0.00
	TS2	-1298.271161	0.180604	-1298.090557	-16.46	-1297.780665	-1297.600061	323.61	326.46	320.84	323.69
	2	-1298.363806	0.186543	-1298.177263	-11.48	-1297.874830	-1297.688287	95.96	119.65	89.21	112.89
	TS3	-1298.327191	0.182405	-1298.144785	-14.57	-1297.838474	-1297.656068	181.24	191.99	173.80	184.55
	3	-1298.383068	0.188065	-1298.195003	-15.48	-1297.893675	-1297.705610	49.39	56.33	43.72	50.67
	1 <sub>eq</sub>	-1374.825102	0.200606	-1374.624496	-26.99	-1374.324852	-1374.124246	0.00	0.00	0.00	0.00
	TS2	-1374.748946	0.205473	-1374.543473	-17.52	-1374.248161	-1374.042688	212.73	252.35	214.13	253.75
	2	-1374.802137	0.207851	-1374.594286	-15.15	-1374.302441	-1374.094590	79.32	128.85	77.86	127.40
	TS3	-1374.805647	0.205160	-1374.600487	-17.25	-1374.306788	-1374.101628	63.04	103.79	59.38	100.13
	3	-1374.823912	0.209709	-1374.614202	-17.11	-1374.324517	-1374.114807	27.03	68.36	24.78	66.12
	1 <sub>eq</sub>	-1451.283289	0.230495	-1451.052795	-21.43	-1450.770405	-1450.539911	0.00	0.00	0.00	0.00
	TS2	-1451.204252	0.226856	-1450.977396	-23.67	-1450.692267	-1450.465411	197.96	188.59	195.60	186.23
	2	-1451.236431	0.225453	-1451.010978	-20.71	-1450.725856	-1450.500403	109.79	112.80	103.73	106.74
	TS3	-1451.250434	0.226265	-1451.024169	-21.85	-1450.73994	-1450.513675	75.16	73.40	98.88	97.13
	3	-1451.266925	0.231677	-1451.035248	-20.51	-1450.756306	-1450.524629	46.07	49.92	40.12	43.97
	1 <sub>eq</sub>	-1527.718428	0.248700	-1527.469728	-26.02	-1527.194640	-1526.945940	0.00	0.00	0.00	0.00
	TS2	-1527.651563	0.246718	-1527.404845	-23.05	-1527.127010	-1526.880292	170.35	182.78	172.36	184.79
	2	-1527.680506	0.249457	-1527.431049	-22.32	-1527.158559	-1526.909102	101.55	117.03	96.72	112.20
	TS3	-1527.673931	0.247214	-1527.426717	-27.10	-1527.152094	-1526.904880	112.93	108.41	107.80	103.29
	3	-1527.690922	0.243807	-1527.447116	-29.42	-1527.17123	-1526.927424	59.37	45.14	48.61	34.39
	1 <sub>eq</sub>	-1604.151565	0.266790	-1603.884775	-31.64	-1603.617546	-1603.350756	0.00	0.00	0.00	0.00
	TS2	-1604.087951	0.268920	-1603.819030	-27.96	-1603.550087	-1603.281166	172.61	188.01	182.71	198.11
	2	-1604.119555	0.271791	-1603.847764	-22.46	-1603.586949	-1603.315158	97.17	135.58	93.46	131.87
	TS3	-1604.132750	0.270190	-1603.862560	-22.20	-1603.59963	-1603.329440	58.33	97.82	55.97	95.46
	3	-1604.146771	0.275234	-1603.871537	-26.14	-1603.612944	-1603.337710	34.76	57.77	34.25	57.26

Table S4. Energies of calculated stationary points for Mech III of oxazepam (OXZ)

Mech III	B3LYP/6-31+G(d)				B2PLYP/aug-TZVPP		B3LYP/6-31+G(d)		B2PLYP/aug-TZVPP		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	SP(Hartree)	G(Hartree)	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
	<b>Cat1'</b>	-1298.721848	0.201957	-1298.519891	-64.39	-1298.236604	-1298.034647	156.17	131.82	144.45	120.10
	<b>Cat1</b>	-1298.754268	0.201761	-1298.552507	-58.91	-1298.267461	-1298.065700	70.53	69.11	62.92	61.50
	<b>Cat2</b> <b>0w</b>	-1298.734673	0.200825	-1298.533847	-68.14	-1298.249668	-1298.048842	119.53	79.48	107.18	67.14
	<b>Cat3</b>	-1298.781843	0.202472	-1298.579372	-58.57	-1298.292137	-1298.089666	0.00	0.00	0.00	0.00
	<b>TS</b>	-1298.672172	0.196228	-1298.475945	-69.22	-1298.184766	-1297.988539	271.55	226.99	265.51	220.95
	<b>Cat3-Cat1</b>										
	<b>Cat1'</b>	-1375.180620	0.221183	-1374.959437	-61.70	-1374.685473	-1374.464290	116.73	100.16	104.40	87.83
	<b>Cat1</b>	-1375.191096	0.221237	-1374.969859	-60.05	-1374.694756	-1374.473519	89.37	79.70	80.17	70.50
	<b>Cat2</b> <b>1w</b>	-1375.192724	0.221733	-1374.970991	-63.43	-1374.696814	-1374.475081	86.40	62.59	76.07	52.26
	<b>Cat3</b>	-1375.224935	0.221037	-1375.003898	-57.74	-1374.725092	-1374.504055	0.00	0.00	0.00	0.00
	<b>Cat1'</b>	-1451.612164	0.242867	-1451.369297	-61.44	-1451.108206	-1450.865339	148.36	136.22	131.04	118.90
	<b>Cat1</b>	-1451.638233	0.241488	-1451.396745	-62.41	-1451.131258	-1450.889770	76.29	60.10	66.90	50.70
	<b>Cat2</b> <b>2w</b>	-1451.637042	0.241813	-1451.395229	-64.47	-1451.130952	-1450.889139	80.27	55.46	68.55	43.74
	<b>Cat3</b>	-1451.665790	0.239987	-1451.425803	-58.54	-1451.155236	-1450.915249	0.00	0.00	0.00	0.00
	<b>Cat1'</b>	-1528.053669	0.260045	-1527.793624	-61.91	-1527.539118	-1527.279073	143.28	134.99	124.75	116.47
	<b>Cat1</b>	-1528.091450	0.265056	-1527.826394	-60.63	-1527.573457	-1527.308401	57.24	54.31	47.75	44.82
	<b>Cat2</b> <b>3w</b>	-1528.081290	0.259249	-1527.822041	-64.50	-1527.564649	-1527.305400	68.67	49.55	55.63	36.51
	<b>Cat3</b>	-1528.105443	0.257247	-1527.848196	-59.93	-1527.583835	-1527.326588	0.00	0.00	0.00	0.00
	<b>Cat1'</b>	-1604.495926	0.277090	-1604.218836	-62.62	-1603.970618	-1603.693528	123.79	127.52	105.52	109.25
	<b>Cat1</b>	-1604.533568	0.283302	-1604.250266	-61.13	-1604.004719	-1603.721417	41.28	51.23	32.30	42.25
	<b>Cat2</b> <b>4w</b>	-1604.536784	0.281527	-1604.255257	-62.57	-1604.006661	-1603.725134	28.17	32.10	22.54	26.47
	<b>Cat3</b>	-1604.541780	0.275793	-1604.265987	-63.51	-1604.009512	-1603.733719	0.00	0.00	0.00	0.00
	<b>Cat1'</b>	<b>Partial optimiaation; C3-O distance fixed during optimisation</b>									

Table S5. Energies of calculated stationary points for Mech IV of oxazepam (OXZ)

Mech IV	B3LYP/6-31+G(d)				B2PLYP/aug-TZVPP		B3LYP/6-31+G(d)		B2PLYP/aug-TZVPP		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	SP(Hartree)	G(Hartree)	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
	<b>1<sub>eq</sub></b>	-1298.402298	0.188485	-1298.213814	-17.14	-1297.910748	-1297.722264	0.00	0.00	0.00	0.00
	<b>TS4<sub>eq</sub></b>	-1298.329559	0.182785	-1298.146775	-26.28	-1297.835163	-1297.652379	176.01	137.77	183.48	145.24
	<b>4<sub>cis</sub></b>	-1298.379567	0.182328	-1298.197239	-13.44	-1297.884284	-1297.701956	43.52	59.00	53.32	68.80
	<b>TS<sub>rot</sub></b> <b>0w</b>	-1298.373813	0.182499	-1298.191314	-14.25	-1297.878497	-1297.695998	59.07	71.17	68.96	81.05
	<b>4<sub>trans</sub></b>	-1298.396380	0.183499	-1298.212880	-8.41	-1297.901096	-1297.717596	2.45	38.98	12.25	48.78
	<b>TS4<sub>ax</sub></b> /										
	<b>TS4<sub>zwt</sub></b>	-1298.329559	0.182785	-1298.146775	-26.28	-1297.835163	-1297.652379	176.01	137.77	183.48	145.24
	<b>1<sub>eq</sub></b>	-1374.825102	0.200606	-1374.624496	-26.99	-1374.324852	-1374.124246	0.00	0.00	0.00	0.00
	<b>TS4<sub>eq</sub></b>	-1374.798456	0.205304	-1374.593152	-26.89	-1374.294162	-1374.088858	82.29	82.71	92.91	93.33
	<b>4<sub>cis</sub></b>	-1374.812015	0.198126	-1374.613889	-19.92	-1374.306613	-1374.108487	27.85	57.43	41.38	70.96
	<b>TS<sub>rot</sub></b> <b>1w</b>	-1374.809049	0.200567	-1374.608482	-19.41	-1374.304692	-1374.104125	42.04	73.76	52.83	84.54
	<b>4<sub>trans</sub></b>	-1374.826242	0.198974	-1374.627268	-15.46	-1374.320892	-1374.121918	-7.28	40.96	6.11	54.35
	<b>TS4<sub>ax</sub></b> /										
	<b>TS4<sub>zwt</sub></b>	-1374.798456	0.205304	-1374.593152	-26.88	-1374.294162	-1374.088858	82.29	82.75	92.91	93.37
	<b>1<sub>eq</sub></b>	-1451.283289	0.230495	-1451.052795	-21.43	-1450.770405	-1450.539911	0.00	0.00	0.00	0.00
	<b>TS4<sub>eq</sub></b>	-1451.240025	0.225786	-1451.014239	-29.13	-1450.724957	-1450.499171	101.23	69.01	106.96	74.75
	<b>4<sub>cis</sub></b>	-1451.236727	0.215210	-1451.021517	-28.44	-1450.722868	-1450.507659	82.12	52.79	84.68	55.35
	<b>TS<sub>rot</sub></b> <b>2w</b>	-1451.242097	0.219148	-1451.022950	-23.91	-1450.727214	-1450.508067	78.36	67.98	83.61	73.23
	<b>4<sub>trans</sub></b>	-1451.257573	0.215516	-1451.042057	-20.44	-1450.742657	-1450.527141	28.19	32.33	33.53	37.67
	<b>TS4<sub>ax</sub></b>	-1451.252635	0.228613	-1451.024022	-21.04	-1450.736165	-1450.507552	75.54	77.18	84.96	86.59
	<b>TS4<sub>zwt</sub></b>	-1451.240025	0.225786	-1451.014239	-29.12	-1450.724957	-1450.499171	101.23	69.05	106.96	74.79
	<b>1<sub>eq</sub></b>	-1527.718428	0.248700	-1527.469728	-26.02	-1527.194640	-1526.945940	0.00	0.00	0.00	0.00
	<b>TS4<sub>eq</sub></b>	-1527.680575	0.248977	-1527.431598	-30.49	-1527.154698	-1526.905721	100.11	81.41	105.59	86.89
	<b>4<sub>cis</sub></b>	-1527.676258	0.236530	-1527.439728	-30.51	-1527.150908	-1526.914378	78.76	59.98	82.87	64.08
	<b>TS<sub>rot</sub></b> <b>3w</b>	-1527.677903	0.239011	-1527.438892	-28.87	-1527.152898	-1526.913887	80.96	69.04	84.16	72.23
	<b>4<sub>trans</sub></b>	-1527.687644	0.233741	-1527.453903	-25.44	-1527.162743	-1526.929002	41.55	43.98	44.47	46.90
	<b>TS4<sub>ax</sub></b>	-1527.686866	0.248884	-1527.437981	-26.04	-1527.159978	-1526.911093	83.35	83.27	91.49	91.41
	<b>TS4<sub>zwt</sub></b>	-1527.671212	0.246793	-1527.424418	-33.41	-1527.144319	-1526.897526	118.96	88.04	127.11	96.19
	<b>1<sub>eq</sub></b>	-1604.151565	0.266790	-1603.884775	-31.64	-1603.617546	-1603.350756	0.00	0.00	0.00	0.00
	<b>TS4<sub>eq</sub></b>	-1604.125306	0.273192	-1603.852114	-29.66	-1603.587232	-1603.314040	85.75	94.03	96.40	104.68
	<b>4<sub>cis</sub></b>	-1604.121781	0.261924	-1603.859857	-31.47	-1603.585730	-1603.323806	65.42	66.13	70.76	71.47
	<b>TS<sub>rot</sub></b> <b>4w</b>	-1604.117858	0.260444	-1603.857414	-30.75	-1603.581647	-1603.321203	71.84	75.56	77.59	81.32
	<b>4<sub>trans</sub></b>	-1604.127000	0.257860	-1603.869140	-29.83	-1603.592445	-1603.334585	41.05	48.62	42.46	50.03
	<b>TS4<sub>ax</sub></b>	-1604.131867	0.275442	-1603.856426	-29.35	-1603.593756	-1603.318315	74.43	84.01	85.18	94.76
	<b>TS4<sub>zwt</sub></b>	-1604.124865	0.270716	-1603.854149	-29.33	-1603.587972	-1603.317256	80.41	90.07	87.95	97.62



Table S6. Energies of calculated stationary points for temazepam (TMZ)

Name	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta pK_{\text{a}}$ (from OXZ 1/An3)
<b>TMZ 1eq 0w</b>	-1337.710451	0.214954	-1337.495496	-15.21	0.00	0.00	
<b>TMZ 1eq 1w</b>	-1414.143632	0.232903	-1413.910729	-20.38	0.00	0.00	
<b>TMZ 1eq 2w</b>	-1490.581003	0.253529	-1490.327474	-23.78	0.00	0.00	
<b>TMZ 1ax 0w</b>	-1337.698337	0.215240	-1337.483097	-15.86	32.55	29.83	
<b>TMZ TS1 0w</b>	-1337.674923	0.215317	-1337.459606	-14.31	94.23	97.99	
<b>TMZ TS1 1w</b>	-1414.107624	0.234337	-1413.873287	-21.05	98.30	95.50	
<b>TMZ TS1 2w</b>	-1490.540780	0.252883	-1490.287897	-25.62	103.91	96.21	
<b>TMZ An1 0w</b>	-1337.157238	0.200513	-1336.956725	-47.12	-75.40	38.57	13.64
<b>TMZ An1 1w</b>	-1413.597313	0.218528	-1413.378785	-49.51	-42.02	58.10	11.64
<b>TMZ An1 2w</b>	-1490.036191	0.238183	-1489.798008	-52.25	-14.98	64.48	13.75
<b>TMZ An2 0w</b>	-1337.126847	0.198842	-1336.928005	-74.36	0.00	0.00	6.88
<b>TMZ An2 1w</b>	-1413.579230	0.216450	-1413.36278	-73.44	0.00	0.00	1.46
<b>TMZ An2 2w</b>	-1490.030557	0.238253	-1489.792304	-71.24	0.00	0.00	2.45
<b>TMZ TS2 0w</b>	-1337.581798	0.207016	-1337.374782	-14.20	316.93	321.16	
<b>TMZ TS2 1w</b>	-1414.052041	0.231996	-1413.820045	-15.93	238.09	256.71	
<b>TMZ TS2 2w</b>	-1490.507915	0.253462	-1490.254453	-21.82	191.72	199.92	
<b>TMZ Cat1 0w</b>	-1338.037200	0.229747	-1337.807452	-60.99	0.00	0.00	
<b>TMZ Cat1 1w</b>	-1414.492846	0.249212	-1414.243635	-57.35	0.00	0.00	
<b>TMZ Cat1 2w</b>	-1490.936584	0.267187	-1490.669397	-57.99	0.00	0.00	
<b>TMZ Cat2 0w</b>	-1338.068500	0.228190	-1337.840309	-54.55	-86.27	-59.32	
<b>TMZ Cat2 1w</b>	-1414.513628	0.247443	-1414.266185	-54.56	-59.20	-47.53	
<b>TMZ Cat2 2w</b>	-1490.953705	0.266219	-1490.687486	-57.16	-47.49	-44.02	
<b>TMZ Cat3 0w</b>	-1338.092247	0.229150	-1337.863097	-55.21	-146.10	-121.91	
<b>TMZ Cat3 1w</b>	-1414.535686	0.248470	-1414.287216	-53.57	-114.42	-98.61	
<b>TMZ Cat3 2w</b>	-1490.977818	0.270249	-1490.707569	-55.98	-100.22	-91.81	
<b>TMZ TS4 0w</b>	-1337.635210	0.209470	-1337.42574	-24.95	183.14	142.39	
<b>TMZ TS4 1w</b>	-1414.102302	0.231717	-1413.870586	-26.77	105.40	78.66	
<b>TMZ TS4 2w</b>	-1490.547115	0.252582	-1490.294533	-27.43	86.49	71.21	

Table S7. Energies of calculated stationary points for lorazepam (LOR)

Lorazepam	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
LOR 1eq 0w	-1757.989517	0.175484	-1757.814033	-18.74	0.00	0.00	
LOR 1eq 1w	-1834.422442	0.193783	-1834.228659	-23.91	0.00	0.00	
LOR 1eq 2w	-1910.855522	0.211381	-1910.644141	-28.55	0.00	0.00	
LOR 1ax 0w	-1757.978691	0.175732	-1757.802959	-19.08	29.07	27.65	
LOR TS1 0w	-1757.968683	0.175678	-1757.793005	-18.54	55.21	56.05	
LOR TS1 1w	-1834.403109	0.196101	-1834.207008	-22.52	56.84	62.66	
LOR TS1 2w	-1910.836599	0.214340	-1910.622259	-27.78	57.45	60.67	
LOR An1 0w	-1757.441634	0.161795	-1757.279839	-49.17	43.54	75.75	12.62
LOR An1 1w	-1833.880468	0.180883	-1833.699584	-52.18	60.02	80.78	10.95
LOR An1 2w	-1910.322118	0.200417	-1910.121701	-53.99	59.23	76.38	12.74
LOR An2 0w	-1757.410674	0.158911	-1757.251763	-76.48	117.25	35.20	5.51
LOR An2 1w	-1833.860391	0.178663	-1833.681729	-76.65	106.90	25.27	1.22
LOR An2 2w	-1910.312930	0.199366	-1910.113564	-74.19	80.59	13.23	1.67
LOR An3 0w	-1757.458602	0.162181	-1757.296421	-56.87	0.00	0.00	-0.66
LOR An3 1w	-1833.903389	0.180944	-1833.722446	-57.14	0.00	0.00	-3.20
LOR An3 2w	-1910.348597	0.204336	-1910.144260	-58.09	0.00	0.00	-0.65
LOR TS2 0w	-1757.863666	0.168816	-1757.694850	-16.70	312.91	321.45	
LOR TS2 1w	-1834.338543	0.193280	-1834.145263	-17.77	218.96	244.65	
LOR TS2 2w	-1910.793771	0.214219	-1910.579552	-24.31	169.58	187.32	
LOR Cat1 0w	-1758.312658	0.191252	-1758.121405	-65.45	0.00	0.00	
LOR Cat1 1w	-1834.770324	0.212723	-1834.557601	-60.43	0.00	0.00	
LOR Cat1 2w	-1911.216508	0.229245	-1910.987262	-59.94	0.00	0.00	
LOR Cat2 0w	-1758.340970	0.189342	-1758.151628	-59.84	-79.35	-55.88	
LOR Cat2 1w	-1834.788340	0.208489	-1834.579851	-58.90	-58.42	-52.02	
LOR Cat2 2w	-1911.232439	0.229387	-1911.003052	-60.26	-41.46	-42.80	
LOR Cat3 0w	-1758.368482	0.190302	-1758.178180	-57.43	-149.06	-115.51	
LOR Cat3 1w	-1834.811064	0.208836	-1834.602228	-57.87	-117.17	-106.46	
LOR Cat3 2w	-1911.252609	0.227275	-1911.025334	-58.86	-99.96	-95.44	
LOR TS4 0w	-1757.917140	0.170282	-1757.746858	-26.38	176.37	144.40	
LOR TS4 1w	-1834.384062	0.192400	-1834.191662	-27.76	97.14	81.03	
LOR TS4 2w	-1910.828175	0.212885	-1910.615290	-28.44	75.75	76.21	

Table S8. Energies of calculated stationary points for lormetazepam (LMZ)

Lormetazepam	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
LMZ 1eq 0w	-1797.297366	0.202327	-1797.095038	-16.58	0.00	0.00	
LMZ 1eq 1w	-1873.731049	0.220109	-1873.51094	-21.47	0.00	0.00	
LMZ 1eq 2w	-1950.163694	0.238427	-1949.925267	-26.67	0.00	0.00	
LMZ 1ax 0w	-1797.288452	0.203113	-1797.085339	-16.18	25.46	27.14	
LMZ An1 0w	-1796.745822	0.188124	-1796.557698	-47.61	-74.18	41.76	13.62
LMZ An1 1w	-1873.185828	0.206861	-1872.978966	-50.1	-46.24	53.71	12.02
LMZ An1 2w	-1949.624922	0.225477	-1949.399445	-52.7	-20.25	63.81	13.86
LMZ An2 0w	-1796.715087	0.185642	-1796.529446	-75.32	0.00	0.00	6.31
LMZ An2 1w	-1873.167358	0.206005	-1872.961353	-73.99	0.00	0.00	2.61
LMZ An2 2w	-1949.618052	0.226318	-1949.391734	-72.79	0.00	0.00	2.68
LMZ Cat1 0w	-1797.624426	0.217724	-1797.406702	-61.46	0.00	0.00	
LMZ Cat1 1w	-1874.081709	0.238885	-1873.842824	-56.75	0.00	0.00	
LMZ Cat1 2w	-1950.524850	0.256879	-1950.267971	-56.68	0.00	0.00	
LMZ Cat2 0w	-1797.654813	0.215805	-1797.439009	-55.58	-84.82	-60.22	
LMZ Cat2 1w	-1874.100064	0.235191	-1873.864873	-55.25	-57.89	-51.61	
LMZ Cat2 2w	-1950.544025	0.255774	-1950.288251	-56.81	-53.25	-53.79	
LMZ Cat3 0w	-1797.678873	0.216807	-1797.462067	-53.98	-145.36	-114.06	
LMZ Cat3 1w	-1874.121310	0.236114	-1873.885196	-54.81	-111.25	-103.13	
LMZ Cat3 2w	-1950.562548	0.254717	-1950.307832	-55.7	-104.65	-100.55	
LMZ TS2 0w	-1797.174228	0.195221	-1796.979007	-14.31	304.64	314.14	
LMZ TS2 1w	-1873.641314	0.220164	-1873.421151	-16.14	235.74	258.04	
LMZ TS2 2w	-1950.096883	0.24091	-1949.855972	-22.46	181.93	199.55	
LMZ TS4 0w	-1797.224296	0.197351	-1797.026945	-24.32	178.78	146.39	
LMZ TS4 1w	-1873.691308	0.219436	-1873.471873	-26.08	102.57	83.28	
LMZ TS4 2w	-1950.135124	0.239845	-1949.895279	-26.79	78.73	78.23	

Table S9. Energies of calculated stationary points for 3-ethyl-carfluzepat (ECF)

Name	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)	
	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
ECF 1eq 0w	-1797.632213	0.286153	-1797.346059	-17.30	0.00	0.00
ECF 1eq 1w	-1874.067118	0.304966	-1873.762151	-21.09	0.00	0.00
ECF 1eq 2w	-1950.499128	0.324014	-1950.175114	-27.36	0.00	0.00
ECF TS2 0w	-1797.534375	0.279823	-1797.254551	-16.27	240.25	244.56
ECF TS2 1w	-1873.985395	0.304389	-1873.681006	-26.26	213.05	191.41
ECF TS2 2w	-1950.464519	0.324208	-1950.140311	-27.52	91.38	90.71

Table S10. Energies of calculated stationary points for 3-cyano-1,4-benzodiazepine (CNZ)

Name	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta pK_{\text{a}}$ (from OXZ 1/An3)
CNZ 1eq 0w	-1315.411152	0.180981	-1315.230171	-16.96	0.00	0.00	
CNZ 1eq 1w	-1391.842239	0.196739	-1391.645501	-23.43	0.00	0.00	
CNZ 1eq 2w	-1468.279159	0.218888	-1468.060270	-25.01	0.00	0.00	
CNZ An1 0w	-1314.891988	0.167229	-1314.724760	-48.65	-19.35	-2.07	-1.55
CNZ An1 1w	-1391.331600	0.183704	-1391.147896	-50.87	-22.08	-2.91	-2.92
CNZ An1 2w	-1467.763264	0.198804	-1467.564459	-56.45	-8.02	-3.12	-3.91
CNZ An2 0w	-1314.884297	0.166906	-1314.717391	-52.78	0.00	0.00	-1.18
CNZ An2 1w	-1391.321736	0.182249	-1391.139488	-55.45	0.00	0.00	-2.41
CNZ An2 2w	-1467.762817	0.201411	-1467.561405	-57.62	0.00	0.00	-3.36
CNZ TS2 0w	-1315.312234	0.174739	-1315.137495	-16.66	243.32	244.58	
CNZ TS2 1w	-1391.777832	0.199721	-1391.578111	-21.86	176.93	183.50	
CNZ TS2 2w	-1468.234272	0.221589	-1468.012683	-29.00	124.94	108.25	

Table S11. Energies of calculated stationary points for 3-ethyl-loflazepat (ELZ)

Name	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol	$\Delta pK_{\text{a}}$ (from OXZ 1/An3)
ELZ 1eq 0w	-1589.614548	0.237891	-1589.376657	-17.65	0.00	0.00	
ELZ 1eq 1w	-1666.049916	0.257907	-1665.79201	-21.6	0.00	0.00	
ELZ 1eq 2w	-1742.496486	0.280271	-1742.216215	-21.63	0.00	0.00	
ELZ An1 0w	-1589.073373	0.222318	-1588.851056	-56.32	6.02	12.51	2.62
ELZ An1 1w	-1665.519726	0.240837	-1665.278889	-54.46	1.24	7.77	0.24
ELZ An1 2w	-1741.962481	0.261532	-1741.700949	-54.8	2.22	19.75	3.77
ELZ An2 0w	-1589.076683	0.223333	-1588.85335	-57.87	0.00	0.00	0.43
ELZ An2 1w	-1665.522765	0.243403	-1665.279362	-56.02	0.00	0.00	-1.12
ELZ An2 2w	-1741.967321	0.265526	-1741.701796	-58.99	0.00	0.00	0.31
ELZ TS2 0w	-1589.517198	0.23216	-1589.285038	-16.49	240.55	245.40	
ELZ TS2 1w	-1665.969496	0.255152	-1665.714345	-21.84	203.91	202.91	
ELZ TS2 2w	-1742.423020	0.277048	-1742.145973	-30.5	184.42	147.31	

Table S12. Energies of calculated stationary points for camazepam (CAM)

Name	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)	
	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
CAM 1eq 0w	-1585.045537	0.287112	-1584.758425	-15.83	0.00	0.00
CAM 1eq 1w	-1661.478975	0.304872	-1661.174103	-20.72	0.00	0.00
CAM 1eq 2w	-1737.91245852	0.324053	-1737.588406	-25.75	0.00	0.00
CAM TS2 0w	-1584.92050367	0.282661	-1584.637843	-14.52	316.59	322.07
CAM TS2 1w	-1661.38651809	0.305396	-1661.081122	-20.35	244.12	245.67
CAM TS2 2w	-1737.86086976	0.328143	-1737.532727	-22.30	146.19	160.62

Table S13. Energies of calculated stationary points for cinazepam (CIN)

Cinazepam	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
CIN 1eq 0w	-4250.082553	0.242702	-4249.839851	-24.95	0.00	0.00	
CIN 1eq 1w	-4326.517717	0.256662	-4326.261056	-28.43	0.00	0.00	
CIN 1eq 2w	-4402.963298	0.285636	-4402.677663	-28.14	0.00	0.00	
CIN An1 0w	-4249.540630	0.227446	-4249.313185	-55.04	17.23	52.83	9.40
CIN An1 1w	-4325.981944	0.246775	-4325.735169	-56.61	23.72	59.49	9.55
CIN An1 2w	-4402.419589	0.266903	-4402.152687	-60.16	38.55	60.97	9.08
CIN An2 0w	-4249.548619	0.228873	-4249.319746	-63.55	0.00	0.00	0.15
CIN An2 1w	-4325.990889	0.246685	-4325.744204	-65.16	0.00	0.00	-0.88
CIN An2 2w	-4402.438389	0.271102	-4402.167369	-65.52	0.00	0.00	-1.60
CIN TS2 0w	-4249.952302	0.236374	-4249.715929	-24.19	325.36	328.54	
CIN TS2 1w	-4326.431762	0.259997	-4326.171766	-27.78	234.43	237.15	
CIN TS2 2w	-4402.887616	0.2823	-4402.605317	-33.92	189.94	165.76	

Table S14. Energies of calculated stationary points for 3-methyl-clonazepam (MCZ)

3-methyl-clonazepam	B3LYP/6-31+G(d)				B3LYP/6-31+G(d)		
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol	$\Delta G_{\text{w}}$ kJ/mol
MCZ 1eq 0w	-1467.001854	0.209016	-1466.792838	-15.71	0.00	0.00	
MCZ 1eq 1w	-1543.433901	0.227880	-1543.206021	-21.8	0.00	0.00	
MCZ 1eq 2w	-1619.863682	0.244231	-1619.619452	-28.97	0.00	0.00	
MCZ An1 0w	-1466.459465	0.193710	-1466.265755	-44.67	41.78	68.93	10.42
MCZ An1 1w	-1542.899394	0.211653	-1542.687741	-47.29	34.23	64.39	8.02
MCZ An1 2w	-1619.334053	0.228049	-1619.106003	-51.71	47.04	67.33	10.58
MCZ An2 0w	-1466.477253	0.195585	-1466.281668	-51.16	0.00	0.00	-1.65
MCZ An2 1w	-1542.913340	0.212563	-1542.700777	-54.50	0.00	0.00	-3.26
MCZ An2 2w	-1619.353613	0.229694	-1619.123919	-56.56	0.00	0.00	-1.22
MCZ TS2 0w	-1466.888316	0.202932	-1466.685384	-12.98	282.12	293.54	
MCZ TS2 1w	-1543.356196	0.225137	-1543.131059	-17.35	196.81	215.43	
MCZ TS2 2w	-1619.806360	0.247155	-1619.559206	-25.36	158.18	173.28	

Table S14. Energies of calculated stationary points on M06-2X/6-31+G(d) for all mechanisms

OXZ	M06-2X/6-31+G(d)				M06-2X/6-31+G(d)			
	Name	SP(Hartree)	TcG(Hartree)	G(Hartree)	$\Delta G_{\text{solv}}$ kcal/mol	$\Delta G_{\text{gas}}$ kJ/mol		$\Delta G_{\text{w}}$ kJ/ mol
	<b>1eq</b>	-1298.035468	0.191700	-1297.843768	-17.15	0.00	0.00	Inversion
	<b>1ax</b> <b>0w</b>	-1298.024649	0.191530	-1297.833119	-17.56	27.96	26.24	
	<b>TS1</b>	-1298.004841	0.191449	-1297.813392	-17.30	79.75	79.12	
	<b>1eq</b> <b>1w</b>	-1374.427992	0.212342	-1374.215650	-20.38	0.00	0.00	
	<b>1eq</b>	-1450.844477	0.234308	-1450.610169	-21.18	0.00	0.00	
	<b>1ax</b> <b>2w</b>	-1450.839197	0.234844	-1450.604353	-22.92	15.27	7.99	
	<b>TS1</b>	-1450.836898	0.234898	-1450.601999	-22.49	21.45	15.97	
	<b>1eq</b> <b>3w</b>	-1527.250809	0.258659	-1526.992150	-21.55	0.00	0.00	
	<b>1eq</b>	-1603.651672	0.279514	-1603.372158	-23.71	0.00	0.00	
	<b>1ax</b> <b>4w</b>	-1603.626373	0.272884	-1603.353489	-30.92	49.02	18.85	
	<b>TS1</b>	-1603.650175	0.281144	-1603.369031	-25.61	8.21	0.26	
	<b>An1</b>	-1297.482332	0.177195	-1297.305137	-50.53	49.14	78.39	Mech I
	<b>An2</b> <b>0w</b>	-1297.452674	0.176105	-1297.276569	-77.11	124.15	42.19	
	<b>An3</b>	-1297.502500	0.178645	-1297.323855	-57.52	0.00	0.00	
	<b>An1</b>	-1373.887317	0.197540	-1373.689777	-52.89	48.91	73.34	
	<b>An2</b> <b>1w</b>	-1373.868964	0.196018	-1373.672946	-75.63	93.10	22.39	
	<b>An3</b>	-1373.907995	0.199589	-1373.708407	-58.73	0.00	0.00	
	<b>An1</b>	-1450.292428	0.216956	-1450.075472	-54.84	62.49	77.59	
	<b>An2</b> <b>2w</b>	-1450.284378	0.217704	-1450.066674	-73.55	85.59	22.41	
	<b>An3</b>	-1450.320419	0.221145	-1450.099274	-58.45	0.00	0.00	
	<b>An1</b>	-1526.703456	0.242115	-1526.461342	-56.77	67.46	63.23	
	<b>An2</b> <b>3w</b>	-1526.698552	0.241220	-1526.457332	-72.63	77.99	7.40	
	<b>An3</b>	-1526.733925	0.246886	-1526.487038	-55.76	0.00	0.00	
	<b>An3</b>	-1603.098390	0.257014	-1602.841376	-59.70	71.37	68.16	
	<b>An2</b> <b>4w</b>	-1603.109223	0.263109	-1602.846114	-72.92	58.93	0.40	
	<b>An1</b>	-1603.136184	0.267623	-1602.868561	-58.93	0.00	0.00	
	<b>TS2</b> <b>0w</b>	-1297.899158	0.183935	-1297.715223	-17.50	337.49	336.03	Mech II
	<b>TS2</b> <b>1w</b>	-1374.348781	0.209593	-1374.139188	-19.38	200.75	204.93	
	<b>TS2</b> <b>2w</b>	-1450.770110	0.231224	-1450.538886	-24.12	187.15	174.85	
	<b>TS2</b> <b>3w</b>	-1527.179617	0.251391	-1526.928225	-25.05	167.83	153.19	
	<b>TS2</b> <b>4w</b>	-1603.576258	0.272649	-1603.303609	-28.24	179.98	161.02	
	<b>Cat2</b> <b>0w</b>	-1298.364390	0.204065	-1298.160325	-68.89	109.91	66.82	Mech III
	<b>Cat1</b> <b>0w</b>	-1298.383895	0.204801	-1298.179094	-59.55	60.64	56.62	
	<b>Cat3</b> <b>0w</b>	-1298.407637	0.205448	-1298.202189	-58.59	0.00	0.00	
	<b>Cat1</b> <b>1w</b>	-1374.786705	0.225104	-1374.561601	-61.09	74.62	59.94	
	<b>Cat2</b> <b>1w</b>	-1374.787543	0.225649	-1374.561894	-63.72	73.85	48.16	
	<b>Cat3</b> <b>1w</b>	-1374.814589	0.224566	-1374.590023	-57.58	0.00	0.00	
	<b>Cat1</b> <b>2w</b>	-1451.201083	0.247032	-1450.954051	-61.06	54.98	43.68	
	<b>Cat2</b> <b>2w</b>	-1451.196249	0.244707	-1450.951542	-64.20	61.56	37.13	
	<b>Cat3</b> <b>2w</b>	-1451.218135	0.243145	-1450.974990	-58.36	0.00	0.00	
	<b>Cat2</b> <b>3w</b>	-1527.603828	0.263429	-1527.340399	-63.50	50.01	35.53	
	<b>Cat1</b> <b>3w</b>	-1527.619443	0.270170	-1527.349274	-60.68	26.71	24.03	
	<b>Cat3</b> <b>3w</b>	-1527.620231	0.260785	-1527.359446	-60.04	0.00	0.00	
	<b>Cat1</b> <b>4w</b>	-1604.023823	0.287821	-1603.736003	-61.17	-3.72	-0.70	
	<b>Cat2</b> <b>4w</b>	-1604.021427	0.285750	-1603.735677	-63.12	-2.86	-8.01	
	<b>Cat3</b> <b>4w</b>	-1604.026940	0.292352	-1603.734588	-61.89	0.00	0.00	

XYZ coordinates for Table S1

**1ax 0w**

C -0.525999 0.156629 -0.007204  
 C 0.547472 -0.859498 0.223882  
 C -1.739244 -0.175376 -0.658163  
 C -1.788786 -2.679335 -0.410921  
 C -0.318649 1.492716 0.390225  
 H 0.599786 1.756628 0.902840  
 C -1.267127 2.471732 0.128246  
 C -2.442463 2.156129 -0.561112  
 C -2.671027 0.840525 -0.941268  
 H -3.595655 0.583546 -1.452127  
 H -3.174807 2.926829 -0.778159  
 N -2.041421 -1.481349 -1.068769  
 C 1.964737 -0.446593 -0.010490  
 C 2.309625 0.487394 -1.002405  
 C 2.989517 -1.048251 0.740491  
 C 3.647714 0.808705 -1.239929  
 C 4.323596 -0.715210 0.512176  
 H 2.721496 -1.776468 1.498985  
 C 4.657535 0.213270 -0.479845  
 H 3.899414 1.522607 -2.019819  
 H 5.104514 -1.180412 1.108095  
 H 5.698368 0.470386 -0.658994  
 O -2.206325 -3.734134 -0.854106  
 Cl -0.984877 4.122378 0.652602  
 C -0.976341 -2.577338 0.895930  
 N 0.352804 -2.076382 0.597761  
 H 1.534872 0.950005 -1.606884  
 H -2.717719 -1.582106 -1.819482  
 O -1.689929 -1.898098 1.922354  
 H -1.723111 -0.945188 1.739840  
 H -0.877254 -3.597263 1.264868

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**1ax 1w**

C -0.211850 0.530516 -0.262662  
 C 0.200765 -0.900071 -0.170893  
 C -1.325240 0.938790 -1.031636  
 C -2.588771 -1.218817 -1.319960  
 C 0.543764 1.514543 0.399545  
 H 1.392347 1.216226 1.004965  
 C 0.219522 2.859838 0.287202  
 C -0.849035 3.270671 -0.512787  
 C -1.612213 2.307560 -1.161666  
 H -2.464003 2.615747 -1.763128  
 H -1.089397 4.324205 -0.611897  
 N -2.141455 0.028703 -1.721235  
 C 1.664381 -1.213732 -0.211651  
 C 2.565557 -0.448951 -0.971787  
 C 2.149015 -2.337350 0.480114  
 C 3.915872 -0.799846 -1.039113  
 C 3.499638 -2.678189 0.424421  
 H 1.449371 -2.937026 1.053379  
 C 4.388551 -1.910922 -0.336489  
 H 4.596559 -0.204616 -1.642355  
 H 3.860043 -3.544665 0.973250  
 H 5.441141 -2.178729 -0.382160

O -3.372808 -1.857532 -2.002378  
 Cl 1.174224 4.060723 1.148032  
 C -2.037319 -1.718243 0.022200  
 N -0.596868 -1.907890 -0.079890  
 H 2.209759 0.411995 -1.529869  
 H -2.649807 0.386183 -2.523865  
 O -2.458006 -0.804936 1.020019  
 H -2.430322 -1.255881 1.889723  
 H -2.480836 -2.702724 0.190919  
 O -2.492375 -2.030017 3.564886  
 H -3.349851 -1.934198 4.007738  
 H -1.828863 -1.709411 4.195379

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**1ax 2w**

C -0.515332 -0.561234 -0.168854  
 C -0.330531 0.906799 0.014791  
 C 0.370727 -1.331085 -0.952508  
 C 2.393050 0.137983 -1.062247  
 C -1.621731 -1.202229 0.415742  
 H -2.302369 -0.628963 1.034894  
 C -1.850176 -2.556789 0.212893  
 C -1.001186 -3.309152 -0.601982  
 C 0.103058 -2.690274 -1.175558  
 H 0.785058 -3.273874 -1.789238  
 H -1.192201 -4.363836 -0.770712  
 N 1.513211 -0.782404 -1.567287  
 C -1.546171 1.778399 -0.020161  
 C -2.643141 1.488903 -0.849229  
 C -1.574357 2.949402 0.756551  
 C -3.738781 2.353204 -0.904786  
 C -2.675647 3.803082 0.712214  
 H -0.723191 3.174374 1.390952  
 C -3.761051 3.509020 -0.120190  
 H -4.573724 2.122110 -1.561231  
 H -2.688283 4.698810 1.327973  
 H -4.618504 4.176270 -0.156019  
 O 3.429957 0.408635 -1.674426  
 Cl -3.231455 -3.329841 0.975060  
 C 2.032425 0.760149 0.298466  
 N 0.797045 1.506544 0.179589  
 H -2.635063 0.596883 -1.468762  
 H 1.870803 -1.269771 -2.383373  
 O 1.985474 -0.244732 1.290062  
 H 2.872954 -0.265815 1.723599  
 H 2.824302 1.479841 0.524596  
 O 4.597372 -0.061513 2.185723  
 H 5.119445 0.238808 1.400769  
 H 5.051435 -0.842392 2.534254  
 O 5.740566 0.781448 -0.169915  
 H 6.111567 1.672530 -0.248517  
 H 4.986831 0.735567 -0.803740

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**1ax 3w**

C -0.321335 -0.538527 0.084020  
 C -0.643783 0.915883 0.048801  
 C 0.991525 -1.022965 -0.117514

C 2.358959 1.025798 0.246242  
 C -1.357692 -1.469175 0.285145  
 H -2.367491 -1.113264 0.455939  
 C -1.104168 -2.833225 0.269695  
 C 0.181526 -3.316250 0.014242  
 C 1.215222 -2.408897 -0.178032  
 H 2.221510 -2.770049 -0.367430  
 H 0.371014 -4.384169 -0.021023  
 N 2.101725 -0.187103 -0.324089  
 C -1.914485 1.342264 -0.619430  
 C -2.427832 0.663690 -1.737823  
 C -2.586018 2.487584 -0.157675  
 C -3.582690 1.119773 -2.377671  
 C -3.746828 2.933513 -0.787904  
 H -2.178961 3.020857 0.695384  
 C -4.249341 2.251384 -1.901461  
 H -3.958910 0.590340 -3.249263  
 H -4.259681 3.815424 -0.412250  
 H -5.152725 2.600967 -2.394883  
 O 3.372694 1.679171 -0.019313  
 Cl -2.419373 -3.966890 0.555431  
 C 1.322196 1.550082 1.245250  
 N 0.090304 1.860023 0.530333  
 H -1.913861 -0.211917 -2.122875  
 H 2.879386 -0.599047 -0.861842  
 O 1.198750 0.596969 2.283609  
 H 0.785879 1.030178 3.059860  
 H 1.713881 2.493554 1.633771  
 O 0.055474 1.746251 4.598570  
 H 0.524003 1.488143 5.407547  
 H -0.876185 1.521057 4.746783  
 O 4.253270 -1.312305 -1.926795  
 H 4.910601 -1.943760 -1.598903  
 H 4.748811 -0.467842 -2.079504  
 O 5.321624 1.185605 -1.911727  
 H 5.240198 1.814652 -2.643363  
 H 4.671631 1.470444 -1.224054

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**1ax 4w**

C 0.193246 0.351515 0.086860  
 C 1.277732 -0.668248 0.042495  
 C -1.166418 0.014156 -0.103767  
 C -1.141958 -2.451100 0.244931  
 C 0.526355 1.704356 0.287789  
 H 1.562472 1.979990 0.449781  
 C -0.454557 2.685249 0.283636  
 C -1.793364 2.367008 0.043262  
 C -2.132359 1.033215 -0.149373  
 H -3.169687 0.765650 -0.326751  
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 N -1.614584 -1.301333 -0.315229  
 C 2.565541 -0.301838 -0.628948  
 C 2.601030 0.541973 -1.751917  
 C 3.769001 -0.862221 -0.167268  
 C 3.809038 0.815883 -2.397565  
 C 4.976433 -0.576263 -0.802995  
 H 3.737886 -1.527461 0.689745  
 C 5.000871 0.263522 -1.921875

H 3.816500 1.460080 -3.273110  
H 5.899762 -1.010564 -0.427684  
H 5.941886 0.483608 -2.419789  
O -1.614403 -3.561078 -0.022344  
Cl 0.002866 4.365229 0.569990  
C 0.018279 -2.308579 1.235666  
N 1.206742 -1.864972 0.517489  
H 1.680206 0.970551 -2.136227  
H -2.486932 -1.395387 -0.857372  
O -0.407824 -1.461104 2.285956  
H 0.190952 -1.586601 3.051470  
H 0.228250 -3.312312 1.613869  
O 1.230605 -1.761538 4.572999  
H 0.711199 -1.824000 5.389619  
H 1.856833 -1.033793 4.710394  
O -4.004001 -1.576567 -1.948550  
H -4.904109 -1.379486 -1.649922  
H -3.969437 -2.559175 -2.070442  
O -3.542832 -4.254937 -1.870530  
H -3.132422 -4.739404 -2.601623  
H -2.834364 -4.118235 -1.194901  
O -4.165070 4.777817 -0.011024  
H -4.061812 5.294214 0.802832  
H -3.969093 5.395493 -0.731932

\*\*\*\*

**1eq 0w**

C -0.547811 0.299111 0.017580  
C -0.996144 1.477258 -0.623279  
C 0.906995 0.013800 0.210141  
C 1.013451 2.938157 -0.439481  
C 1.338668 2.244043 0.894120  
O 1.710603 3.831992 -0.895679  
N 1.770120 0.893894 0.580277  
N -0.099264 2.459323 -1.090552  
C -2.368552 1.666830 -0.854913  
C -3.303081 0.728877 -0.433990  
H -4.361905 0.888144 -0.609590  
C -2.862219 -0.413438 0.240922  
C -1.507716 -0.632900 0.455026  
H -1.181155 -1.535443 0.959757  
H -2.703014 2.571034 -1.357306  
O 2.321874 2.958570 1.576563  
C 1.405317 -1.372607 -0.037737  
C 0.816289 -2.211981 -0.998268  
C 2.525333 -1.837323 0.673876  
C 1.335638 -3.485460 -1.242511  
H -0.038213 -1.865543 -1.572345  
C 3.035156 -3.112608 0.436838  
H 2.985430 -1.182929 1.407324  
C 2.442450 -3.941347 -0.522478  
H 0.875557 -4.118738 -1.996598  
H 3.895807 -3.461825 1.001454  
H 2.841886 -4.935247 -0.707404  
H -0.369168 2.997746 -1.907596  
H 0.443134 2.233928 1.534067  
Cl -4.034809 -1.587938 0.812198  
H 2.844925 3.444316 0.910639

\*\*\*\*

**1eq 1w**

C -0.184894 0.463193 0.265835  
C -0.331347 1.715598 -0.376542  
C 1.119272 -0.270049 0.264883  
C 2.038064 2.462223 -0.559681  
C 2.326229 1.714090 0.752725  
O 2.900701 3.085733 -1.158609  
N 2.259632 0.294353 0.458173  
N 0.746231 2.353485 -1.022424  
C -1.593091 2.333007 -0.421329  
C -2.697733 1.752952 0.191325  
H -3.665945 2.242008 0.161759  
C -2.540239 0.540552 0.871360  
C -1.308302 -0.102413 0.897036  
H -1.209968 -1.055114 1.405640  
H -1.698141 3.292073 -0.922917  
H 1.579930 1.996696 1.510902  
O 3.574040 2.084597 1.249678  
H 4.118942 2.369027 0.491360  
C 1.113290 -1.744166 0.027320  
C 0.141572 -2.364026 -0.775399  
C 2.137523 -2.532140 0.581424  
C 0.192592 -3.737792 -1.021037  
H -0.651649 -1.774902 -1.225675  
C 2.181016 -3.904713 0.344834  
H 2.893762 -2.049955 1.192466  
C 1.209094 -4.512705 -0.457931  
H -0.561386 -4.198635 -1.653541  
H 2.973648 -4.502190 0.787677  
H 1.245075 -5.583082 -0.643289  
H 0.538718 2.947006 -1.819279  
Cl -3.912159 -0.174988 1.693151  
O -3.527870 -0.249433 -2.858048  
H -3.662085 0.608497 -3.287524  
H -2.828481 -0.100342 -2.204497

\*\*\*\*

**1eq 2w**

C 0.410590 0.555271 -0.336557  
C -0.838447 1.161279 -0.064911  
C 0.559005 -0.925348 -0.464658  
C -2.398132 -0.651782 -0.664546  
C -1.413394 -1.078849 -1.763704  
O -3.444072 -1.285131 -0.481703  
N -0.276422 -1.680208 -1.089606  
N -2.029552 0.421868 0.081700  
C -0.908424 2.550909 0.135338  
C 0.222042 3.349583 0.026134  
H 0.155623 4.422725 0.172614  
C 1.446888 2.754457 -0.292359  
C 1.546046 1.380027 -0.456988  
H 2.508313 0.931518 -0.678088  
H -1.867831 3.000276 0.373604  
H -1.108816 -0.201364 -2.352800  
O -2.023674 -1.966312 -2.649041  
H -2.683665 -2.474806 -2.141694  
C 1.742907 -1.585298 0.162769

C 2.319641 -1.096290 1.346976  
C 2.267742 -2.754170 -0.415607  
C 3.396315 -1.760291 1.938916  
H 1.916284 -0.205963 1.820629  
C 3.350064 -3.408724 0.170163  
H 1.812823 -3.136888 -1.323697  
C 3.918242 -2.914312 1.349618  
H 3.824367 -1.375719 2.860991  
H 3.752088 -4.305724 -0.293863  
H 4.761363 -3.426569 1.806095  
H -2.738755 0.803421 0.728692  
Cl 2.876837 3.757864 -0.471283  
O -5.149875 -1.029158 1.695921  
H -6.050472 -1.333580 1.514002  
H -4.610426 -1.235189 0.896811  
O -4.004915 1.431800 1.923967  
H -4.608394 2.168982 1.750215  
H -4.573132 0.625218 1.996973

\*\*\*\*

**1eq 3w**

C 0.858039 0.527204 -0.315649  
C -0.390704 1.103271 0.014575  
C 1.038915 -0.952048 -0.408543  
C -1.942975 -0.751281 -0.463467  
C -0.996938 -1.196523 -1.590918  
O -2.983449 -1.377479 -0.236833  
N 0.188982 -1.746686 -0.960088  
N -1.546701 0.333038 0.252298  
C -0.495962 2.495579 0.182492  
C 0.600996 3.323500 -0.017856  
H 0.509257 4.398277 0.100963  
C 1.823400 2.756391 -0.393089  
C 1.957880 1.381485 -0.526572  
H 2.919411 0.956525 -0.793051  
H -1.456243 2.918458 0.464081  
H -0.744665 -0.332612 -2.224023  
O -1.629276 -2.130992 -2.411837  
H -2.279222 -2.604471 -1.858945  
C 2.271323 -1.564276 0.173124  
C 2.903545 -1.020569 1.303826  
C 2.788144 -2.743577 -0.391339  
C 4.025369 -1.641479 1.857777  
H 2.509481 -0.120267 1.766335  
C 3.914888 -3.355354 0.155656  
H 2.291056 -3.168354 -1.257654  
C 4.537558 -2.806838 1.282515  
H 4.496576 -1.214236 2.739179  
H 4.309132 -4.261280 -0.297659  
H 5.415329 -3.285773 1.708920  
H -2.226526 0.722609 0.929365  
Cl 3.207930 3.797924 -0.685159  
O -7.446964 -0.264390 -0.191053  
H -7.313002 -0.078516 -1.133171  
H -8.024463 -1.042200 -0.151983  
O -5.105071 -0.507526 1.436978  
H -4.447395 -0.955094 0.862685  
H -5.909064 -0.383115 0.893062  
O -3.453037 1.529876 2.007312

H -3.303289 1.575584 2.963288  
H -4.195645 0.876477 1.879141

\*\*\*\*

**1eq 4w**

C 0.724208 0.377007 -0.490343  
C -0.579283 0.925279 -0.494025  
C 1.005676 -0.976346 0.072038  
C -1.973504 -1.076665 -0.186456  
C -0.916960 -1.883727 -0.956188  
O -2.991967 -1.643253 0.233944  
N 0.250939 -2.003975 -0.111666  
N -1.702548 0.233633 0.005569  
C -0.784643 2.239074 -0.949756  
C 0.269993 2.995217 -1.444072  
H 0.101783 4.004146 -1.806419  
C 1.550619 2.434179 -1.485747  
C 1.781436 1.153321 -1.004086  
H 2.785274 0.743428 -1.020733  
H -1.787651 2.654660 -0.916534  
H -0.681016 -1.379295 -1.904920  
O -1.442164 -3.148413 -1.275466  
H -2.184864 -3.308364 -0.658493  
C 2.229733 -1.171056 0.905944  
C 2.744317 -0.143763 1.714618  
C 2.858023 -2.428561 0.925036  
C 3.859962 -0.369118 2.524250  
H 2.263028 0.829801 1.727809  
C 3.978236 -2.648182 1.724776  
H 2.452319 -3.223932 0.308019  
C 4.483171 -1.619351 2.527845  
H 4.239758 0.432815 3.151997  
H 4.459545 -3.622814 1.721518  
H 5.356275 -1.792065 3.151960  
H -2.456197 0.818239 0.424757  
Cl 2.885108 3.369077 -2.142034  
O -5.292127 -0.416789 1.249117  
H -4.534636 -0.957701 0.927164  
H -6.043100 -0.638065 0.678902  
O -3.372398 2.798232 3.715274  
H -3.476692 2.084516 4.363810  
H -3.959235 3.511773 4.009239  
O -3.746057 1.861508 1.035303  
H -3.597546 2.223103 1.932932  
H -4.471796 1.201226 1.129054  
O -2.057156 -3.000708 -4.048150  
H -1.635463 -3.718487 -4.542103  
H -1.886298 -3.193351 -3.103886

\*\*\*\*

**TS1 0w**

C 1.536104 1.281274 -0.091151  
C -0.873107 2.714791 0.047154  
C 0.317969 0.569762 0.053275  
C 1.501936 2.684995 -0.218661  
C 0.320355 3.406700 -0.158735  
C -0.869349 1.332728 0.148019  
H 2.438251 3.221088 -0.354554

H 0.328276 4.487475 -0.254509  
H -1.809803 0.823174 0.306878  
N 2.822714 0.734455 -0.088275  
C 3.350750 -0.497318 0.245094  
O 4.532444 -0.575686 0.544332  
C 0.183423 -0.916487 0.124681  
N 1.079700 -1.827772 0.223727  
C 2.513812 -1.778324 0.165483  
H 2.881003 -2.402198 0.991466  
C -1.213156 -1.490684 0.063525  
C -3.739096 -2.710257 -0.092750  
C -1.690072 -2.273624 1.122939  
C -2.009733 -1.331774 -1.080473  
C -3.262026 -1.945085 -1.161028  
C -2.950710 -2.870672 1.050181  
H -1.065650 -2.417061 2.000292  
H -1.645821 -0.737348 -1.915065  
H -3.863586 -1.824262 -2.058249  
H -3.312837 -3.467340 1.883483  
H -4.717172 -3.180498 -0.152357  
Cl -2.386264 3.596766 0.174045  
H 3.564939 1.428670 -0.085444  
O 2.898520 -2.346549 -1.086777  
H 2.301661 -3.101766 -1.234644

\*\*\*\*

**TS1 1w**

C -1.282367 1.425637 -0.294364  
C 1.217322 2.676201 -0.061584  
C -0.112486 0.625126 -0.271574  
C -1.165942 2.822223 -0.150451  
C 0.060689 3.454791 -0.028662  
C 1.128080 1.298715 -0.179588  
H -2.070736 3.425294 -0.143760  
H 0.117636 4.533053 0.077464  
H 2.042372 0.722525 -0.205266  
N -2.592193 0.980914 -0.497266  
C -3.194378 -0.228759 -0.747137  
O -4.367063 -0.254860 -1.094637  
C -0.076290 -0.863875 -0.359148  
N -1.023772 -1.710209 -0.545471  
C -2.448046 -1.555703 -0.569204  
H -2.822678 -2.186657 -1.384219  
C 1.266871 -1.540735 -0.209081  
C 3.676649 -2.948432 0.097435  
C 1.792355 -2.285867 -1.272412  
C 1.953347 -1.513264 1.014688  
C 3.147922 -2.220839 1.167693  
C 2.997034 -2.976997 -1.123594  
H 1.250651 -2.326668 -2.213415  
H 1.547658 -0.948998 1.851017  
H 3.664043 -2.202476 2.124076  
H 3.399289 -3.544160 -1.959129  
H 4.610131 -3.492458 0.215770  
Cl 2.792550 3.443703 0.046861  
H -3.273890 1.727500 -0.599526  
O -2.940686 -2.067549 0.682520  
H -2.482264 -2.916072 0.825905  
O -2.238077 -0.423465 2.941459

H -3.065322 -0.289259 3.426194  
H -2.476451 -0.981862 2.174571

\*\*\*\*

**TS1 2w**

C 0.341079 -1.816849 -0.487749  
C -2.353090 -2.218237 0.171367  
C -0.489915 -0.690496 -0.276812  
C -0.210293 -3.108576 -0.404115  
C -1.542429 -3.323461 -0.082960  
C -1.836261 -0.935197 0.074922  
H 0.432246 -3.967803 -0.581643  
H -1.938879 -4.331372 -0.018848  
H -2.487291 -0.096639 0.280714  
N 1.710439 -1.790103 -0.787103  
C 2.706952 -0.855401 -0.658795  
O 3.875998 -1.218641 -0.667419  
C -0.061388 0.732548 -0.387288  
N 1.101184 1.236533 -0.579998  
C 2.395739 0.646569 -0.708900  
H 2.774285 0.953526 -1.697045  
C -1.132265 1.790417 -0.262957  
C -3.025915 3.849437 -0.054300  
C -2.081650 1.983297 -1.275933  
C -1.135055 2.636797 0.853022  
C -2.083886 3.656485 0.960141  
C -3.019816 3.013407 -1.174745  
H -2.082938 1.334098 -2.148514  
H -0.395811 2.488664 1.635679  
H -2.083308 4.302441 1.834358  
H -3.744522 3.161828 -1.971158  
H -3.760130 4.646710 0.026800  
Cl -4.035370 -2.450312 0.614350  
H 2.127145 -2.711685 -0.888425  
O 3.230111 1.240715 0.300153  
H 3.001821 2.187847 0.311197  
O 6.148830 0.724491 0.336945  
H 6.256555 -0.161184 -0.041826  
H 5.185231 0.862228 0.297690  
O 1.961017 -0.136912 2.443304  
H 2.474021 -0.577053 3.137145  
H 2.603023 0.397026 1.936392

\*\*\*\*

**TS1 3w**

C -1.069786 0.674901 0.077721  
C 0.640192 2.896302 0.190865  
C 0.320969 0.486350 -0.114139  
C -1.559335 1.970119 0.344081  
C -0.726318 3.076219 0.405531  
C 1.147896 1.631916 -0.060878  
H -2.626037 2.098215 0.507709  
H -1.131237 4.061268 0.613849  
H 2.211816 1.520916 -0.221629  
N -2.067728 -0.300081 0.016533  
C -2.105992 -1.645183 -0.207478  
O -3.191337 -2.228964 -0.222170  
C 0.984917 -0.816785 -0.390343



N 0.483416 -1.975284 -0.607824  
C -0.852948 -2.478735 -0.510492  
H -1.078685 -2.968849 -1.468663  
C 2.495495 -0.825313 -0.432459  
C 5.295759 -0.966738 -0.481500  
C 3.174182 -0.949712 -1.650246  
C 3.224827 -0.780922 0.764112  
C 4.619552 -0.855948 0.737491  
C 4.570138 -1.013528 -1.675047  
H 2.608376 -1.002074 -2.577024  
H 2.697356 -0.703403 1.711825  
H 5.177035 -0.830329 1.670385  
H 5.088655 -1.105720 -2.626118  
H 6.381310 -1.019933 -0.500364  
Cl 1.723508 4.279342 0.241246  
H -3.022562 0.065835 0.142130  
O -0.828009 -3.476464 0.525761  
H -0.009230 -3.983179 0.376914  
O -0.137715 -1.873709 2.804661  
H -0.796218 -1.864656 3.514537  
H -0.453797 -2.538220 2.159104  
O -7.079627 0.942797 -1.254803  
H -6.985546 1.700342 -1.852125  
H -7.865082 1.122262 -0.715489  
O -4.889027 -0.005684 0.326980  
H -4.751327 -0.955460 0.139658  
H -5.605858 0.300265 -0.263586

\*\*\*\*

#### TS1 4w

C -0.689067 1.152129 0.106874  
C 1.488742 2.912569 0.199703  
C 0.617399 0.641394 -0.084745  
C -0.868739 2.530385 0.333101  
C 0.199843 3.413190 0.380644  
C 1.689766 1.559596 -0.026472  
H -1.876749 2.907342 0.483736  
H 0.033840 4.470448 0.559722  
H 2.700268 1.197154 -0.159166  
N -1.886316 0.424914 0.093932  
C -2.216650 -0.887239 0.018821  
O -3.406910 -1.218769 0.125956  
C 0.958335 -0.782944 -0.351424  
N 0.201556 -1.807462 -0.484456  
C -1.202897 -1.994116 -0.295288  
H -1.588381 -2.457059 -1.215611  
C 2.424370 -1.126147 -0.485406  
C 5.117995 -1.866124 -0.700994  
C 3.070252 -1.076625 -1.726326  
C 3.128505 -1.552330 0.648724  
C 4.472514 -1.918662 0.538176  
C 4.413716 -1.447152 -1.833327  
H 2.522664 -0.754949 -2.609212  
H 2.617875 -1.600135 1.607712  
H 5.013560 -2.249528 1.421150  
H 4.907395 -1.410614 -2.801180  
H 6.163093 -2.153135 -0.784630  
Cl 2.865709 4.000883 0.259620  
H -2.734399 1.002204 0.216848

O -1.346662 -2.937179 0.784500  
H -0.705272 -3.645348 0.592228  
O 0.113667 -1.606226 2.880457  
H -0.348178 -1.458663 3.718737  
H -0.499042 -2.127361 2.323434  
O -6.327455 2.405479 -1.470875  
H -7.185699 2.696992 -1.126521  
H -6.523768 1.846270 -2.238433  
O -4.514477 1.410501 0.502845  
H -4.642396 0.442807 0.489713  
H -5.110656 1.772808 -0.184247  
O -4.208233 -3.893130 -0.584263  
H -3.987356 -2.986607 -0.289920  
H -3.784473 -4.462769 0.074443

\*\*\*\*

XYZ coordinates for Table S2

**An1 0w**

C -0.479961 0.334726 0.153119  
 C -1.811202 0.112239 0.588689  
 C 0.482378 -0.766711 0.003949  
 C -2.213166 -2.276380 0.280703  
 C -1.052167 -2.539242 -0.526128  
 O -3.178054 -3.074322 0.344748  
 N 0.122149 -1.975094 -0.450650  
 N -2.170331 -1.156375 1.143067  
 C -2.754451 1.143896 0.577844  
 C -2.416592 2.446227 0.193633  
 H -3.142750 3.251764 0.226456  
 C -1.108832 2.666072 -0.234979  
 C -0.165449 1.648658 -0.277519  
 H 0.829236 1.859705 -0.652516  
 H -3.768501 0.933621 0.914195  
 O -1.136978 -3.727649 -1.251729  
 H -2.005827 -4.098990 -1.001017  
 C 1.932515 -0.533341 0.105252  
 C 2.487408 0.496700 0.904657  
 C 2.854252 -1.387800 -0.552121  
 C 3.866473 0.676149 1.018492  
 H 1.825025 1.150469 1.465593  
 C 4.229208 -1.204077 -0.438338  
 H 2.454448 -2.202230 -1.147474  
 C 4.757644 -0.166938 0.344852  
 H 4.247095 1.478255 1.649652  
 H 4.900903 -1.877973 -0.969110  
 H 5.832963 -0.026735 0.433618  
 H -3.045079 -1.122666 1.658701  
 Cl -0.642255 4.299398 -0.765989

\*\*\*\*

**An1 1w**

C -0.003187 0.484417 -0.052251  
 C 1.352659 0.690733 -0.401833  
 C -0.580777 -0.868999 0.061842  
 C 2.448886 -1.434687 0.032875  
 C 1.387615 -2.046468 0.759296  
 O 3.632536 -1.892523 0.083138  
 N 0.096607 -1.895732 0.572799  
 N 2.135563 -0.405597 -0.880630  
 C 1.915615 1.970766 -0.373434  
 C 1.154685 3.097136 -0.044208  
 H 1.585404 4.092974 -0.063174  
 C -0.176970 2.893470 0.310716  
 C -0.747354 1.626869 0.327217  
 H -1.779818 1.510236 0.635939  
 H 2.959987 2.091925 -0.654170  
 O 1.779561 -3.132702 1.542477  
 H 2.735268 -3.227876 1.364253  
 C -2.020929 -1.098410 -0.162061  
 C -2.787042 -0.308666 -1.052121  
 C -2.689730 -2.176023 0.469186  
 C -4.139819 -0.565627 -1.280207  
 H -2.307538 0.504244 -1.590707  
 C -4.040098 -2.427326 0.242785

H -2.114141 -2.810602 1.135346  
 C -4.785927 -1.624105 -0.632406  
 H -4.690152 0.063094 -1.978722  
 H -4.519923 -3.259743 0.755981  
 H -5.840560 -1.824108 -0.809826  
 H 2.985718 -0.097874 -1.347528  
 Cl -1.170013 4.294359 0.771395  
 O 5.437773 -0.281794 -1.181822  
 H 4.871870 -0.964483 -0.732908  
 H 5.854208 0.205080 -0.456109

\*\*\*\*

**An1 2w**

C -0.105897 -0.798520 0.030048  
 C 1.206326 -1.241778 0.319283  
 C -0.457981 0.636048 -0.016624  
 C 2.628318 0.697979 -0.063833  
 C 1.659154 1.499720 -0.722400  
 O 3.866242 0.973828 -0.132819  
 N 0.364349 1.564432 -0.493396  
 N 2.181973 -0.318920 0.805265  
 C 1.542575 -2.596296 0.222416  
 C 0.589934 -3.563085 -0.112560  
 H 0.847783 -4.616438 -0.149081  
 C -0.701052 -3.126881 -0.400241  
 C -1.047554 -1.782090 -0.351173  
 H -2.056805 -1.481221 -0.607495  
 H 2.562100 -2.902069 0.447743  
 O 2.205897 2.572857 -1.447440  
 H 3.167887 2.514004 -1.279286  
 C -1.842911 1.078516 0.248554  
 C -2.671846 0.429478 1.192056  
 C -2.380187 2.215004 -0.401084  
 C -3.962190 0.885564 1.465977  
 H -2.287909 -0.431137 1.733438  
 C -3.668351 2.668390 -0.126751  
 H -1.762196 2.729805 -1.130361  
 C -4.476491 2.008957 0.809670  
 H -4.566060 0.363441 2.206445  
 H -4.048742 3.542303 -0.653047  
 H -5.481701 2.365127 1.024273  
 H 2.983539 -0.782024 1.230603  
 Cl -1.934672 -4.320780 -0.856102  
 O 5.248068 -0.748376 1.465615  
 H 4.897426 -0.077659 0.821301  
 H 5.486347 -0.234844 2.251103  
 O 0.697699 4.852438 -0.516461  
 H 0.017771 4.287729 -0.115283  
 H 1.291417 4.185632 -0.920880

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**An1 3w**

C -0.235185 -0.670714 0.061068  
 C 1.152491 -0.776107 0.302555  
 C -0.972789 0.605549 0.220917  
 C 1.968940 1.517125 0.151790  
 C 0.793843 2.096977 -0.380815  
 O 3.084042 2.131561 0.096280

N -0.461484 1.774430 -0.140967  
 N 1.862250 0.318991 0.890379  
 C 1.841324 -1.968461 0.052174  
 C 1.174857 -3.099636 -0.426070  
 H 1.703532 -4.033944 -0.585455  
 C -0.187022 -2.989854 -0.695227  
 C -0.881980 -1.806386 -0.475415  
 H -1.937848 -1.754800 -0.714813  
 H 2.906006 -2.017557 0.273456  
 O 0.992982 3.353237 -0.977279  
 H 1.953617 3.516327 -0.900731  
 C -2.399732 0.612481 0.602094  
 C -2.984942 -0.422272 1.368570  
 C -3.233990 1.706259 0.265777  
 C -4.325811 -0.377913 1.754105  
 H -2.374311 -1.262796 1.685607  
 C -4.572027 1.745577 0.647483  
 H -2.798998 2.530837 -0.289572  
 C -5.137998 0.701894 1.393384  
 H -4.735002 -1.193102 2.348699  
 H -5.182045 2.600716 0.360643  
 H -6.183360 0.735378 1.692441  
 H 2.782915 0.035268 1.213196  
 Cl -1.058587 -4.395421 -1.341810  
 O -0.896643 3.670476 -3.104410  
 H -0.185343 3.667071 -2.429516  
 H -1.500821 2.986000 -2.778720  
 O 5.390775 1.292160 1.156906  
 H 4.544873 1.632090 0.740821  
 H 5.414318 1.675900 2.045312  
 O 5.271407 -1.466804 0.921857  
 H 5.375069 -0.492172 1.045193  
 H 5.667655 -1.649168 0.057467

\*\*\*\*

**An1 4w**

C -0.492950 0.919018 -0.087268  
 C 0.845507 1.370556 -0.074588  
 C -0.871607 -0.408697 -0.625792  
 C 2.177587 -0.649921 -0.273371  
 C 1.131910 -1.576976 -0.060547  
 O 3.398298 -0.995402 -0.157508  
 N -0.131429 -1.492132 -0.430122  
 N 1.850362 0.629769 -0.770596  
 C 1.189656 2.574922 0.549298  
 C 0.222944 3.387187 1.146908  
 H 0.489676 4.337489 1.597666  
 C -1.094298 2.933973 1.151360  
 C -1.451539 1.724266 0.567345  
 H -2.483047 1.394375 0.612557  
 H 2.229217 2.895881 0.539395  
 O 1.572338 -2.863031 0.300041  
 H 2.547386 -2.799213 0.330623  
 C -2.201886 -0.625824 -1.231450  
 C -2.925845 0.416794 -1.854263  
 C -2.779995 -1.916701 -1.272764  
 C -4.164150 0.188090 -2.456561  
 H -2.502043 1.416372 -1.886569  
 C -4.017110 -2.142016 -1.870157

H -2.225040 -2.742942 -0.840796  
C -4.728321 -1.091214 -2.465486  
H -4.686443 1.017659 -2.929936  
H -4.431538 -3.148674 -1.873190  
H -5.693896 -1.269116 -2.933428  
H 2.699037 1.169981 -0.917379  
Cl -2.344852 3.919802 1.930972  
O 5.193384 0.970042 -0.407850  
H 4.583185 0.182053 -0.307369  
H 5.616709 1.082315 0.455854  
O 7.161919 0.556317 -2.393207  
H 6.855317 -0.246814 -2.838795  
H 6.470604 0.739617 -1.715903  
O -0.129992 -3.749537 4.619108  
H -0.246710 -3.925552 3.656750  
H 0.213718 -2.844871 4.653348  
O -0.428069 -4.067962 1.829940  
H -1.147420 -3.527798 1.467215  
H 0.358811 -3.755017 1.328277

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#### An2 0w

C 0.588127 0.161750 0.030192  
C 1.748921 -0.325206 -0.622939  
C -0.611425 -0.714257 0.221446  
C 1.449042 -2.833497 -0.426497  
C 0.756782 -2.622540 0.983695  
O 1.744444 -3.890224 -0.953101  
N -0.567336 -1.948520 0.566060  
N 1.841222 -1.635757 -1.087315  
C 2.819543 0.560441 -0.868189  
C 2.779678 1.885682 -0.451055  
H 3.617480 2.550666 -0.637445  
C 1.650505 2.340540 0.232786  
C 0.568939 1.500055 0.460943  
H -0.310008 1.878348 0.972390  
H 3.705368 0.186484 -1.377556  
O 0.618821 -3.665995 1.724074  
C -1.966162 -0.116840 -0.035675  
C -2.184519 0.892755 -0.989120  
C -3.078173 -0.622537 0.662970  
C -3.470711 1.383163 -1.236373  
H -1.345263 1.289006 -1.554378  
C -4.359293 -0.127583 0.424055  
H -2.906771 -1.419621 1.380230  
C -4.564393 0.879889 -0.527676  
H -3.615713 2.158126 -1.986712  
H -5.203521 -0.529290 0.981098  
H -5.564865 1.264479 -0.715272  
H 2.524057 -1.808630 -1.819253  
H 1.368177 -1.783558 1.438416  
Cl 1.596857 4.017811 0.802830

\*\*\*\*

#### An2 1w

C 0.712318 -0.449963 -0.025701  
C 0.853034 -1.711342 -0.657178  
C -0.611880 0.243790 0.020020

C -1.537926 -2.543619 -0.715773  
C -1.803274 -1.803225 0.650569  
O -2.300985 -3.276134 -1.315045  
N -1.732611 -0.338026 0.243023  
N -0.227735 -2.375201 -1.236377  
C 2.136970 -2.286114 -0.760914  
C 3.258709 -1.662906 -0.227949  
H 4.238260 -2.124313 -0.306765  
C 3.100721 -0.441876 0.431529  
C 1.853912 0.161610 0.523025  
H 1.753579 1.122150 1.017387  
H 2.243529 -3.250338 -1.253413  
O -2.898999 -2.131274 1.273879  
C -0.642389 1.723977 -0.229574  
C 0.232318 2.355888 -1.129485  
C -1.612343 2.506422 0.422822  
C 0.138095 3.728846 -1.376188  
H 0.981908 1.768588 -1.653255  
C -1.700199 3.877678 0.183977  
H -2.293497 2.014486 1.111214  
C -0.825900 4.496711 -0.717730  
H 0.817469 4.196154 -2.086235  
H -2.453897 4.465596 0.703337  
H -0.897018 5.566035 -0.905413  
H -0.006293 -3.066534 -1.946522  
H -0.860342 -1.998667 1.237419  
Cl 4.514660 0.348210 1.145595  
O -4.727739 -0.124840 1.424223  
H -4.113122 -0.918243 1.447566  
H -4.328592 0.380829 0.699906

\*\*\*\*

#### An2 2w

C 0.746733 -0.598036 -0.128708  
C 0.345876 -1.766198 -0.821315  
C -0.128966 0.614561 -0.091822  
C -2.147152 -1.427439 -1.009681  
C -2.123483 -0.696160 0.374413  
O -3.131184 -1.692884 -1.678816  
N -1.400660 0.590456 0.072058  
N -0.887749 -1.853426 -1.472522  
C 1.235900 -2.854668 -0.911190  
C 2.486223 -2.820332 -0.305811  
H 3.158005 -3.670229 -0.374154  
C 2.854125 -1.681678 0.414751  
C 2.006771 -0.585194 0.496527  
H 2.318285 0.298302 1.043425  
H 0.925040 -3.747142 -1.449858  
O -3.304352 -0.528456 0.936043  
C 0.514255 1.958496 -0.273071  
C 1.652325 2.149679 -1.074121  
C -0.070139 3.081417 0.339441  
C 2.192884 3.425927 -1.258297  
H 2.111762 1.299284 -1.570633  
C 0.474090 4.352804 0.163199  
H -0.959714 2.929876 0.942921  
C 1.609196 4.532463 -0.636752  
H 3.068980 3.553058 -1.890826  
H 0.011213 5.207740 0.651306

H 2.032124 5.525263 -0.774694  
H -0.956689 -2.515440 -2.238934  
H -1.424130 -1.311494 0.998078  
Cl 4.426763 -1.637414 1.221432  
O -5.551302 -0.109383 -0.610926  
H -4.787776 -0.170029 0.024768  
H -5.216444 -0.670430 -1.328130  
O -3.302405 0.198606 3.518492  
H -3.812797 1.018881 3.456473  
H -3.281865 -0.127722 2.565457

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#### An2 3w

C 0.652791 -0.745087 -0.177704  
C -0.243420 -1.540151 -0.933132  
C 0.504905 0.740046 -0.117831  
C -2.205894 0.013336 -1.227642  
C -1.898395 0.621930 0.182074  
O -3.152864 0.289868 -1.944321  
N -0.614638 1.358988 -0.021777  
N -1.310404 -0.985455 -1.645740  
C -0.022215 -2.928597 -1.025726  
C 1.040370 -3.538431 -0.371029  
H 1.190869 -4.611063 -0.441807  
C 1.897966 -2.751248 0.401539  
C 1.716119 -1.378583 0.491924  
H 2.402327 -0.780101 1.081421  
H -0.714535 -3.535320 -1.604737  
O -2.858201 1.387473 0.682912  
C 1.744737 1.582316 -0.175216  
C 2.859290 1.229231 -0.953343  
C 1.778873 2.790726 0.543434  
C 3.978247 2.064562 -1.019088  
H 2.847192 0.304208 -1.523799  
C 2.900615 3.617863 0.486309  
H 0.912681 3.063578 1.140040  
C 4.004930 3.260080 -0.296174  
H 4.827234 1.780176 -1.637110  
H 2.913220 4.544505 1.055769  
H 4.878004 3.907525 -0.341263  
H -1.673444 -1.532067 -2.420287  
H -1.663177 -0.272133 0.817575  
Cl 3.235944 -3.517157 1.265635  
O -5.082053 -2.073311 1.297648  
H -4.401335 -1.885284 1.960529  
H -5.232085 -1.190406 0.866348  
O -5.290981 0.454432 0.183643  
H -4.406253 0.864620 0.454665  
H -5.177586 0.399307 -0.779089  
O -1.953255 3.811221 1.595836  
H -2.336533 2.918683 1.363255  
H -1.457021 4.015290 0.789197

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#### An2 4w

C -1.005482 -0.341458 0.417765  
C -0.692807 -1.277950 1.433123  
C -0.033445 0.723512 0.021343

C 1.819384 -1.131718 1.518418  
C 1.815619 -0.842284 -0.015557  
O 2.803470 -1.269964 2.224905  
N 1.228448 0.532612 -0.120440  
N 0.545371 -1.281370 2.085027  
C -1.672744 -2.202178 1.844039  
C -2.929145 -2.236397 1.252107  
H -3.670772 -2.962232 1.570185  
C -3.214479 -1.338198 0.220807  
C -2.275331 -0.400466 -0.185942  
H -2.522547 0.305596 -0.971328  
H -1.428785 -2.917098 2.626426  
O 3.000798 -0.955593 -0.604501  
C -0.556130 2.109044 -0.209197  
C -1.643638 2.627025 0.513938  
C 0.089205 2.939239 -1.141737  
C -2.074791 3.940512 0.311350  
H -2.144606 2.009085 1.254067  
C -0.345660 4.247727 -1.348292  
H 0.940017 2.545174 -1.688588  
C -1.430334 4.754153 -0.624124  
H -2.910730 4.328070 0.889492  
H 0.168548 4.874926 -2.072342  
H -1.766355 5.776301 -0.783604  
H 0.572090 -1.670158 3.022288  
H 1.061842 -1.553926 -0.434067  
Cl -4.795349 -1.390782 -0.562144  
O 2.946539 -2.485477 -2.713950  
H 2.982401 -1.833484 -1.926951  
H 3.573177 -3.182344 -2.470996  
O 0.380393 -3.521360 -3.016781  
H 1.306562 -3.172682 -2.953834  
H -0.136076 -2.914395 -2.466277  
O 5.070190 0.186527 0.680183  
H 4.845491 -0.155277 1.560458  
H 4.363820 -0.251831 0.119158  
O 3.523497 2.582394 0.408227  
H 4.215779 1.893482 0.527749  
H 2.753906 2.049799 0.129619

\*\*\*\*

**An3 0w**

C -0.464961 0.454162 -0.016249  
C 0.870524 -0.153104 -0.212533  
C -0.610960 1.764549 0.562039  
C 1.590395 2.636771 0.505892  
C -1.615106 -0.282413 -0.385676  
H -1.496059 -1.267415 -0.826190  
C -2.882636 0.239709 -0.214899  
C -3.062705 1.507522 0.362430  
C -1.950662 2.233542 0.742502  
H -2.062858 3.212345 1.200759  
H -4.063401 1.906700 0.504650  
N 0.374467 2.570651 1.045845  
C 1.055668 -1.624328 0.025982  
C 0.332976 -2.318780 1.010395  
C 2.019303 -2.331319 -0.714624  
C 0.563557 -3.677244 1.245815  
C 2.245112 -3.688873 -0.486500

H 2.592113 -1.788746 -1.460381  
C 1.516900 -4.370693 0.495430  
H -0.001879 -4.191690 2.020122  
H 2.991948 -4.217236 -1.075920  
H 1.692811 -5.429449 0.674528  
O 2.568031 3.263029 0.967804  
Cl -4.305770 -0.694493 -0.729237  
C 1.835013 1.903209 -0.856396  
H 1.002228 2.101702 -1.549513  
N 1.930760 0.493230 -0.568377  
O 3.020491 2.387181 -1.434804  
H 3.447934 2.863001 -0.684846  
H -0.404004 -1.787928 1.605888

\*\*\*\*

**An3 1w**

C 0.235610 -0.629039 -0.153325  
C -0.655273 -1.470649 -0.906264  
C -0.025240 0.818985 0.007787  
C -2.577239 -0.120734 -1.191231  
C -2.345878 0.489512 0.232294  
O -3.549292 0.351355 -1.823065  
N -1.194663 1.346417 0.160209  
N -1.766932 -1.090337 -1.600072  
C -0.281920 -2.844996 -1.029433  
C 0.850108 -3.374657 -0.440970  
H 1.091222 -4.428778 -0.547305  
C 1.690209 -2.528464 0.301044  
C 1.399733 -1.184129 0.429200  
H 2.064999 -0.543992 1.000048  
H -0.942345 -3.475312 -1.618485  
O -3.500356 1.226995 0.586565  
C 1.124468 1.783780 -0.019098  
C 2.254522 1.572195 -0.826293  
C 1.056977 2.966292 0.738008  
C 3.287046 2.512924 -0.874559  
H 2.317771 0.672788 -1.431758  
C 2.090777 3.902117 0.697456  
H 0.174482 3.137287 1.346718  
C 3.212761 3.679747 -0.109176  
H 4.148311 2.333306 -1.514565  
H 2.021539 4.807731 1.296666  
H 4.019068 4.409554 -0.141677  
H -2.201974 -0.307632 0.977450  
Cl 3.138870 -3.201844 1.078330  
H -3.963519 1.317626 -0.284524  
O -5.329909 -0.116181 2.253600  
H -4.671457 0.418193 1.750236  
H -5.551224 -0.836637 1.645182

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**An3 2w**

C 0.380714 0.544790 -0.315329  
C -0.918389 1.089448 -0.056817  
C 0.595233 -0.918593 -0.426958  
C -2.358669 -0.740331 -0.485264  
C -1.413497 -1.212354 -1.626684  
O -3.361230 -1.475789 -0.272633

N -0.221119 -1.737373 -0.998982  
N -2.075673 0.379511 0.162485  
C -1.011515 2.502994 0.090452  
C 0.079727 3.340863 -0.052937  
H -0.030211 4.416475 0.051102  
C 1.335174 2.781734 -0.333171  
C 1.489488 1.412632 -0.443793  
H 2.471202 0.996288 -0.645863  
H -1.989676 2.914650 0.322278  
O -2.053557 -2.190942 -2.403296  
C 1.831281 -1.526163 0.167564  
C 2.418182 -1.018188 1.338208  
C 2.397022 -2.669315 -0.423195  
C 3.540119 -1.632842 1.900886  
H 1.984486 -0.147005 1.820299  
C 3.522148 -3.278240 0.132697  
H 1.929367 -3.072098 -1.316345  
C 4.100515 -2.761971 1.298072  
H 3.972698 -1.229210 2.813708  
H 3.949055 -4.158529 -0.343419  
H 4.977286 -3.237419 1.732621  
H -1.163489 -0.364044 -2.282737  
Cl 2.737750 3.848486 -0.541693  
H -2.801120 -2.483352 -1.837034  
O -5.525133 -0.980458 1.345286  
H -4.698770 -1.195000 0.836425  
H -6.156631 -0.716216 0.660406  
O -4.143381 1.513551 1.988755  
H -4.751414 0.747624 1.995574  
H -3.415769 1.190920 1.409948

\*\*\*\*

**An3 3w**

C 0.571787 0.447372 -0.498874  
C -0.844828 0.648892 -0.470978  
C 1.163948 -0.905466 -0.356593  
C -1.695395 -1.543346 -0.766489  
C -0.506118 -1.874226 -1.710112  
O -2.497922 -2.492899 -0.550656  
N 0.674681 -1.977478 -0.880784  
N -1.805024 -0.319320 -0.271271  
C -1.311669 1.990332 -0.554860  
C -0.458135 3.068544 -0.707088  
H -0.849965 4.078771 -0.779857  
C 0.923994 2.839468 -0.760908  
C 1.432462 1.559659 -0.639957  
H 2.505842 1.402126 -0.666021  
H -2.384371 2.150284 -0.497181  
O -0.755354 -3.074380 -2.393441  
C 2.413841 -1.076965 0.454775  
C 2.673194 -0.296810 1.593544  
C 3.333991 -2.080556 0.105923  
C 3.821261 -0.512113 2.360884  
H 1.964653 0.471134 1.889765  
C 4.484900 -2.289545 0.865645  
H 3.121159 -2.695174 -0.763317  
C 4.734817 -1.505022 1.997432  
H 3.997788 0.095792 3.245411  
H 5.188833 -3.066621 0.575188

H 5.631639 -1.668302 2.591187  
H -0.384996 -1.075128 -2.457886  
Cl 2.027357 4.210202 -0.979653  
H -1.471299 -3.496980 -1.871198  
O -4.834716 -2.444563 0.854892  
H -3.943770 -2.487899 0.412236  
H -5.464484 -2.611741 0.138606  
O -4.339973 0.353212 0.966662  
H -4.691340 -0.553719 1.098628  
H -3.445203 0.189292 0.573736  
O -5.113992 2.459179 2.587686  
H -5.669072 2.879395 1.915213  
H -4.750737 1.667236 2.118762

\*\*\*\*

**An3 4w**

C 0.682981 0.459926 -0.405178  
C -0.702622 0.808555 -0.333448  
C 1.171973 -0.873123 0.024361  
C -1.759231 -1.288683 -0.024484  
C -0.685768 -1.958392 -0.925381  
O -2.618486 -2.076309 0.463119  
N 0.550024 -1.983796 -0.185110  
N -1.721569 0.019595 0.160175  
C -1.060893 2.132153 -0.710137  
C -0.136450 3.049034 -1.178077  
H -0.446880 4.048154 -1.468643  
C 1.210890 2.672050 -1.267139  
C 1.618352 1.411862 -0.871308  
H 2.667655 1.142242 -0.930169  
H -2.106030 2.413214 -0.619854  
O -1.107027 -3.269122 -1.243366  
C 2.472216 -0.973964 0.764070  
C 2.893778 0.021987 1.660248  
C 3.273723 -2.117348 0.605156  
C 4.084808 -0.120651 2.377053  
H 2.278735 0.904420 1.810327  
C 4.467544 -2.255665 1.313123  
H 2.936931 -2.893723 -0.074809  
C 4.879234 -1.256822 2.202722  
H 4.388202 0.656744 3.074580  
H 5.078181 -3.144723 1.171360  
H 5.809303 -1.364886 2.756451  
H -0.571745 -1.399789 -1.866715  
Cl 2.401104 3.829234 -1.886011  
H -1.816607 -3.448085 -0.583194  
O -4.725707 -1.445915 2.093093  
H -3.917075 -1.687351 1.566947  
H -5.465030 -1.783601 1.566897  
O -4.106399 1.216423 1.309067  
H -4.483740 0.420251 1.741092  
H -3.260399 0.879138 0.921331  
O -4.651579 3.799779 2.146361  
H -5.267262 3.994675 1.425328  
H -4.368598 2.870941 1.959279  
O -2.050653 -3.774670 -3.863683  
H -1.653859 -3.655859 -2.971189  
H -2.804139 -3.166339 -3.868501

\*\*\*\*

**TS An3 -> An4 2w**

C -0.912124 -0.568126 -0.026970  
C -0.787364 -1.934042 0.467447  
C 0.231657 0.301637 -0.167646  
C 1.577715 -2.307035 0.564546  
C 1.717206 -1.586064 -0.834008  
N 1.425161 -0.165069 -0.469362  
N 0.299386 -2.551003 0.945223  
C -2.022589 -2.674454 0.572878  
C -3.247425 -2.152208 0.245161  
H -4.149773 -2.750582 0.336062  
C -3.331196 -0.815694 -0.216191  
C -2.203576 -0.044934 -0.336434  
H -2.286274 0.971199 -0.707027  
H -1.935070 -3.692204 0.941812  
C 0.122852 1.774141 0.036690  
C 0.844819 2.660706 -0.781074  
C -0.664641 2.300034 1.076557  
C 0.769916 4.038166 -0.570298  
H 1.471181 2.267362 -1.574930  
C -0.732970 3.677195 1.289210  
H -1.210070 1.622236 1.726342  
C -0.019322 4.551351 0.462804  
H 1.336094 4.708888 -1.211613  
H -1.340005 4.066629 2.103090  
H -0.074291 5.625196 0.627015  
O 2.580072 -2.629234 1.202779  
O 4.809511 -0.932355 -0.177931  
H 4.304632 0.311995 -0.034969  
O 3.715150 1.264327 -0.020913  
H 2.278109 0.452976 -0.332423  
H 3.788584 1.621619 0.876378  
H 4.685210 -1.433437 0.644933  
O 2.885150 -1.716734 -1.495964  
H 3.788091 -1.424747 -0.891589  
H 0.880248 -1.908644 -1.471561  
Cl -4.916784 -0.155181 -0.654256

\*\*\*\*

**An4 2w**

C -0.923578 -0.566830 -0.041420  
C -0.743658 -1.937729 0.425409  
C 0.193234 0.327126 -0.218629  
C 1.634623 -2.228466 0.502013  
C 1.756834 -1.580571 -0.955027  
N 1.382497 -0.128212 -0.555475  
N 0.370444 -2.513015 0.888000  
C -1.951145 -2.723002 0.536382  
C -3.200025 -2.231929 0.255046  
H -4.080637 -2.861061 0.351910  
C -3.338091 -0.885100 -0.163570  
C -2.238965 -0.076509 -0.298267  
H -2.364170 0.944393 -0.643586  
H -1.822464 -3.746849 0.875599  
C 0.065133 1.798048 -0.014879  
C 0.736668 2.693989 -0.865299  
C -0.683257 2.317631 1.056791  
C 0.655628 4.071031 -0.653871

H 1.322258 2.306163 -1.693499  
C -0.758939 3.694521 1.269927  
H -1.192069 1.634019 1.729884  
C -0.092619 4.576814 0.413109  
H 1.181032 4.747950 -1.323020  
H -1.335332 4.077984 2.108664  
H -0.153701 5.650122 0.578309  
O 2.642073 -2.463189 1.181742  
O 4.884004 -1.113876 0.026776  
H 4.326543 0.472124 0.132688  
O 3.823252 1.346493 0.140129  
H 2.207624 0.488892 -0.463540  
H 3.761256 1.592031 1.074889  
H 4.445784 -1.621373 0.739361  
O 2.892600 -1.640294 -1.591051  
H 4.237731 -1.356169 -0.719818  
H 0.868019 -1.915816 -1.532333  
Cl -4.957585 -0.261825 -0.534719

XYZ coordinates for Table S3

**2 0w**

C -0.387624 0.426176 0.110157  
 C -1.660099 0.589211 0.692482  
 C 0.263226 -0.915089 -0.055711  
 C -2.641591 -1.562948 0.284795  
 C -1.713503 -2.137049 -0.518549  
 O -3.936516 -1.977933 0.334518  
 N -0.361104 -1.989741 -0.435076  
 N -2.336388 -0.554497 1.208227  
 C -2.230354 1.860921 0.799284  
 C -1.557596 2.990748 0.331639  
 H -1.997200 3.977716 0.431893  
 C -0.317270 2.826208 -0.280231  
 C 0.263095 1.564687 -0.394459  
 H 1.233164 1.463790 -0.867859  
 H -3.209893 1.971551 1.258512  
 O -2.180626 -3.143752 -1.361481  
 H -1.417371 -3.706796 -1.576265  
 C 1.740300 -1.017774 0.102896  
 C 2.431373 -0.226645 1.038474  
 C 2.472608 -1.951494 -0.653977  
 C 3.810064 -0.365660 1.212447  
 H 1.886181 0.488416 1.647710  
 C 3.850086 -2.079951 -0.488983  
 H 1.944936 -2.570353 -1.372510  
 C 4.526549 -1.288425 0.446733  
 H 4.322521 0.247882 1.949125  
 H 4.399588 -2.798075 -1.092683  
 H 5.600799 -1.391341 0.576715  
 H -3.143928 -0.329038 1.779800  
 Cl 0.536830 4.229688 -0.908272  
 H -4.020920 -2.752797 -0.252138

\*\*\*\*

**2 1w**

C -0.325286 0.615579 -0.164310  
 C 0.608514 1.457976 -0.796409  
 C -0.102334 -0.857693 -0.037954  
 C 2.670234 0.226256 -0.554224  
 C 2.259682 -0.775396 0.271363  
 O 3.930106 0.661972 -0.747914  
 N 1.045169 -1.395765 0.247551  
 N 1.755151 0.875043 -1.406089  
 C 0.381612 2.836029 -0.865008  
 C -0.767426 3.401535 -0.310160  
 H -0.948519 4.469121 -0.380685  
 C -1.672446 2.571876 0.348504  
 C -1.459389 1.197372 0.426745  
 H -2.181842 0.571424 0.938471  
 H 1.107105 3.473883 -1.364412  
 O 3.204481 -1.426219 1.080829  
 H 2.794505 -2.279327 1.308828  
 C -1.273530 -1.773891 -0.120189  
 C -2.357866 -1.494791 -0.971573  
 C -1.296718 -2.970044 0.620930  
 C -3.429682 -2.383678 -1.079570  
 H -2.354927 -0.587039 -1.567951

C -2.372433 -3.850034 0.522404  
 H -0.460474 -3.196664 1.274465  
 C -3.444736 -3.562329 -0.330238  
 H -4.251803 -2.153764 -1.752643  
 H -2.376697 -4.763027 1.112846  
 H -4.281969 -4.251052 -0.409157  
 H 2.252530 1.512454 -2.019729  
 Cl -3.112487 3.265717 1.084281  
 H 5.083881 -1.151901 1.153657  
 O 5.811724 -0.659039 0.723387  
 H 6.230059 -0.119534 1.411188  
 H 4.618518 0.156972 -0.240158

\*\*\*\*

**2 2w**

C 0.889348 0.600251 0.146006  
 C 0.072444 1.593718 0.717389  
 C 0.416902 -0.806790 -0.027226  
 C -2.150968 0.754657 0.306949  
 C -1.868243 -0.307027 -0.500794  
 O -3.318647 1.410282 0.413475  
 N -0.785307 -1.128394 -0.405224  
 N -1.199066 1.218786 1.238600  
 C 0.528490 2.911885 0.816130  
 C 1.798068 3.267573 0.358251  
 H 2.156039 4.287427 0.454137  
 C 2.593090 2.290636 -0.237186  
 C 2.149936 0.974882 -0.349671  
 H 2.788321 0.232814 -0.815640  
 H -0.112404 3.667684 1.264075  
 O -2.855992 -0.772585 -1.378605  
 H -2.510457 -1.613961 -1.722499  
 C 1.398516 -1.918825 0.106091  
 C 2.453850 -1.851501 1.033904  
 C 1.262931 -3.088339 -0.665199  
 C 3.343851 -2.917119 1.185093  
 H 2.568797 -0.967993 1.655182  
 C 2.158694 -4.146035 -0.522859  
 H 0.446120 -3.152505 -1.376856  
 C 3.204281 -4.067206 0.404666  
 H 4.145879 -2.846781 1.915684  
 H 2.043489 -5.035018 -1.138340  
 H 3.901191 -4.893864 0.516704  
 H -1.619625 1.940554 1.815374  
 Cl 4.186331 2.720642 -0.850138  
 H -4.780095 -0.267079 -1.422437  
 O -5.344200 0.419145 -1.020603  
 H -6.003639 -0.044304 -0.462638  
 H -4.064372 1.036507 -0.144219  
 O -7.288514 -0.785560 0.651380  
 H -8.180549 -0.427069 0.524889  
 H -7.104024 -0.714883 1.600844

\*\*\*\*

**2 3w**

C -1.014771 0.621012 0.316680  
 C -0.193981 1.479556 1.072552  
 C -0.758412 -0.850300 0.226062

C 1.893567 0.254212 1.191806  
 C 1.619225 -0.736801 0.297369  
 H 1.247427 1.581345 2.529012  
 O 3.100236 0.654163 1.606518  
 N 0.426843 -1.371037 0.118321  
 N 0.856016 0.927061 1.859107  
 C -0.442384 2.855414 1.091796  
 C -1.502706 3.404374 0.368996  
 H -1.701393 4.470641 0.401153  
 C -2.293113 2.558967 -0.405798  
 C -2.055510 1.186555 -0.439061  
 H -2.687609 0.548934 -1.046751  
 H 0.195932 3.505650 1.685331  
 O 2.710830 -1.374275 -0.322712  
 C -1.915865 -1.781328 0.120963  
 C -1.808644 -2.970782 -0.623785  
 C -3.122834 -1.523752 0.795905  
 C -2.874607 -3.864747 -0.699837  
 H -0.878023 -3.180351 -1.141470  
 C -4.186562 -2.426283 0.729340  
 H -3.225005 -0.621770 1.392378  
 C -4.070081 -3.598087 -0.021990  
 H -2.775214 -4.771724 -1.291291  
 H -5.106267 -2.212133 1.267964  
 H -4.900554 -4.297000 -0.079728  
 H 3.365395 -0.553353 -1.808392  
 H 3.878955 0.098766 1.303892  
 O 3.860171 -0.101448 -2.530469  
 H 5.511515 -1.451106 1.233408  
 O 5.448905 -0.491839 1.117169  
 H 3.630530 -0.556294 -3.353700  
 H 2.433323 -2.300158 -0.449463  
 H 5.830833 -0.302645 0.221495  
 Cl -3.617381 3.228959 -1.351305  
 O 6.353311 0.024294 -1.417598  
 H 5.517475 0.021795 -1.946475  
 H 6.750590 0.899706 -1.536428

\*\*\*\*

**2 4w**

C -1.184758 0.611302 0.391715  
 C -0.237477 1.214418 1.241397  
 C -1.268051 -0.871579 0.223340  
 C 1.506301 -0.461889 1.382130  
 C 1.064072 -1.320565 0.416841  
 H 1.104881 0.917850 2.757236  
 O 2.736674 -0.381192 1.886169  
 N -0.229124 -1.646713 0.144627  
 N 0.606639 0.395469 2.043323  
 C -0.163872 2.608271 1.336120  
 C -1.021477 3.425233 0.598168  
 H -0.972301 4.505313 0.690068  
 C -1.934675 2.828284 -0.268179  
 C -2.017785 1.442106 -0.377064  
 H -2.740210 1.000161 -1.054058  
 H 0.566165 3.061090 2.002980  
 O 2.012147 -2.195260 -0.151153  
 C -2.599433 -1.502979 0.007379  
 C -2.720902 -2.650811 -0.797916

C -3.754983 -1.002869 0.634441  
C -3.956401 -3.269299 -0.978192  
H -1.832392 -3.047300 -1.278993  
C -4.991003 -1.630032 0.462406  
H -3.684739 -0.129093 1.275900  
C -5.099086 -2.762581 -0.347952  
H -4.030575 -4.148401 -1.613823  
H -5.868987 -1.232578 0.965407  
H -6.062181 -3.246889 -0.487334  
H 3.090925 -1.776628 -1.480995  
H 3.459419 -0.890441 1.397116  
O 3.905686 -1.562094 -1.998968  
H 4.805688 -1.681830 -0.138223  
O 4.915855 -1.350224 0.771216  
H 3.927501 -2.159008 -2.761777  
H 1.596444 -3.076685 -0.166593  
H 5.479250 -0.543945 0.674025  
Cl -3.005860 3.837086 -1.233660  
O 6.284142 0.969180 0.113873  
H 5.872643 1.115108 -0.772320  
H 7.242977 0.985427 -0.019779  
O 4.909188 1.030429 -2.278487  
H 4.461239 0.154441 -2.248092  
H 4.208904 1.692881 -2.373198

\*\*\*\*

**3 0w**

C -0.477142 -0.426570 -0.018039  
C -0.637765 -1.706776 0.581179  
C 0.866235 0.182078 -0.222206  
C 1.520978 -2.565269 0.436027  
C 1.780404 -1.889398 -0.905368  
O 2.566071 -3.230478 0.952024  
N 1.908497 -0.478678 -0.604159  
N 0.411906 -2.490967 1.069327  
C -1.942571 -2.195151 0.799462  
C -3.061993 -1.486455 0.390651  
H -4.058770 -1.887093 0.545356  
C -2.891573 -0.238201 -0.221572  
C -1.625824 0.296614 -0.403063  
H -1.514295 1.272977 -0.861912  
H -2.049017 -3.155919 1.293941  
O 2.903119 -2.370223 -1.587273  
H 3.696126 -2.067587 -1.112783  
C 1.049981 1.643209 0.028863  
C 0.335592 2.312873 1.036403  
C 1.994375 2.361765 -0.724560  
C 0.562517 3.668127 1.286117  
H -0.386814 1.771208 1.640033  
C 2.211041 3.717406 -0.482255  
H 2.550763 1.842483 -1.498441  
C 1.496532 4.375314 0.524925  
H 0.009399 4.169286 2.076210  
H 2.936722 4.262413 -1.080524  
H 1.666824 5.432089 0.714184  
Cl -4.303252 0.664776 -0.753209  
H 0.922598 -2.096032 -1.560973  
H 2.300687 -3.549308 1.835890

\*\*\*\*

**3 1w**

C 0.065529 0.590182 -0.214743  
C -1.161315 1.188717 0.183860  
C 0.197811 -0.881639 -0.399877  
C -2.680629 -0.546127 -0.212149  
C -1.915126 -0.999615 -1.451713  
O -3.716903 -1.307933 0.115227  
N -0.708131 -1.622441 -0.945164  
N -2.328263 0.477579 0.490918  
C -1.199157 2.583707 0.386068  
C -0.090452 3.384575 0.157020  
H -0.144523 4.459474 0.297301  
C 1.106346 2.786778 -0.256557  
C 1.192725 1.413009 -0.420184  
H 2.132216 0.965143 -0.725257  
H -2.133283 3.026632 0.719044  
O -2.635719 -1.864336 -2.279654  
H -2.844728 -2.667705 -1.773072

C 1.441033 -1.565729 0.066761  
C 2.132758 -1.135097 1.211281  
C 1.906149 -2.699831 -0.620985  
C 3.262326 -1.823990 1.658529  
H 1.777815 -0.271089 1.765470  
C 3.041268 -3.378779 -0.180601  
H 1.365710 -3.036227 -1.500124  
C 3.722699 -2.943907 0.961530  
H 3.780057 -1.485509 2.552247  
H 3.396011 -4.247844 -0.728740  
H 4.606592 -3.475024 1.305453  
H -3.569758 0.537725 2.048801  
Cl 2.516400 3.791450 -0.559527  
H -1.694638 -0.116431 -2.067231  
H -4.104297 -0.994298 0.979505  
O -4.291864 -0.018077 2.424239  
H -5.067109 0.553788 2.530347

\*\*\*\*

**3 2w**

C 0.363346 0.557326 -0.339599  
C -0.914336 1.135837 -0.109648  
C 0.542758 -0.915410 -0.472248  
C -2.349770 -0.635617 -0.641765  
C -1.421073 -1.077306 -1.772625  
O -3.390505 -1.424062 -0.461485  
N -0.278263 -1.678780 -1.111847  
N -2.096422 0.401543 0.088223  
C -1.008323 2.535365 0.036051  
C 0.103461 3.356258 -0.086762  
H 0.008572 4.433503 0.005807  
C 1.353716 2.776914 -0.333085  
C 1.488855 1.401122 -0.439626  
H 2.467025 0.968082 -0.618737  
H -1.984642 2.967445 0.236081  
O -2.015947 -1.955127 -2.681867  
H -2.343979 -2.727334 -2.190118  
C 1.730119 -1.567215 0.156671  
C 2.291057 -1.082102 1.349992

C 2.276472 -2.722739 -0.428484  
C 3.371918 -1.736964 1.944543  
H 1.873270 -0.199721 1.825992  
C 3.362383 -3.368848 0.160127  
H 1.836890 -3.101381 -1.345786  
C 3.913924 -2.878546 1.349099  
H 3.788598 -1.354448 2.872705  
H 3.780971 -4.255270 -0.309569  
H 4.760409 -3.383574 1.807396  
H -3.067461 1.043810 1.525346  
Cl 2.767862 3.807075 -0.501969  
H -1.135707 -0.193478 -2.359455  
O -3.692498 1.296976 2.256081  
H -4.732873 -0.068453 1.979202  
O -5.049921 -0.908679 1.556639  
H -5.966695 -0.760392 1.280183  
H -3.975349 -1.179093 0.323017  
H -3.175977 1.289384 3.075992

\*\*\*\*

**3 3w**

C 0.388402 -0.309001 0.046670  
C -0.696961 -1.183644 -0.233343  
C 0.168922 1.094558 0.494649  
C -2.492330 -0.039394 0.735279  
C -1.606893 0.412343 1.896496  
O -3.711755 0.456136 0.769449  
N -0.751857 1.439876 1.330408  
N -2.047983 -0.803799 -0.210232  
C -0.412075 -2.495551 -0.666729  
C 0.888901 -2.958906 -0.792020  
H 1.086368 -3.979341 -1.103841  
C 1.948601 -2.089508 -0.505730  
C 1.708220 -0.782451 -0.108733  
H 2.541376 -0.119414 0.098058  
H -1.244477 -3.157099 -0.886887  
H -1.029304 -0.448410 2.259322  
O -2.318898 0.878726 3.002264  
H -2.915761 1.587103 2.706561  
C 1.052593 2.176455 -0.032502  
C 1.563891 2.137100 -1.340598  
C 1.342991 3.287876 0.777493  
C 2.346354 3.186394 -1.827814  
H 1.335023 1.295085 -1.987563  
C 2.133889 4.328701 0.293387  
H 0.940650 3.319762 1.785089  
C 2.637688 4.281971 -1.011264  
H 2.725434 3.147303 -2.845740  
H 2.359436 5.176988 0.934486  
H 3.253278 5.094671 -1.388223  
Cl 3.605699 -2.662742 -0.662690  
H -4.266757 0.282548 -0.056233  
O 2.298570 -3.483457 2.778758  
H 1.896147 -2.814673 2.203197  
H 3.129995 -3.713076 2.335293  
O -5.292730 0.125505 -1.336307  
H -5.508751 0.946115 -1.803866  
H -4.801008 -0.454632 -1.974554  
O -3.521034 -1.462817 -2.566208

H -3.717562 -2.410038 -2.619871  
H -2.948476 -1.333202 -1.765836

\*\*\*\*

**3 4w**

C -1.038647 0.584769 0.483999  
C 0.141511 1.373226 0.562359  
C -1.020600 -0.880322 0.747178  
C 1.595774 -0.057611 1.702132  
C 0.450975 -0.579755 2.568144  
O 2.755805 -0.660460 1.918451  
N -0.327842 -1.429706 1.688355  
N 1.424620 0.859299 0.811484  
C 0.058178 2.749560 0.267855  
C -1.150002 3.354311 -0.046054  
H -1.198911 4.419137 -0.249935  
C -2.309367 2.571483 -0.101770  
C -2.256019 1.207228 0.138042  
H -3.161459 0.613360 0.076779  
H 0.970045 3.338746 0.300353  
O 0.868888 -1.263683 3.713153  
H 1.408893 -2.022541 3.434063  
C -1.841177 -1.786561 -0.110365  
C -2.048674 -1.519289 -1.473992  
C -2.379997 -2.961858 0.441053  
C -2.776882 -2.408149 -2.267968  
H -1.625058 -0.624928 -1.921616  
C -3.116961 -3.841849 -0.350167  
H -2.212255 -3.170342 1.493001  
C -3.317291 -3.568402 -1.707835  
H -2.919729 -2.193006 -3.323737  
H -3.537660 -4.741239 0.092292  
H -3.891403 -4.255510 -2.324265  
H 2.715629 1.599222 -0.439902  
Cl -3.847890 3.328306 -0.489463  
H -0.131385 0.277364 2.932864  
O 3.534680 1.824651 -0.939985  
H 4.481659 0.761021 -0.213876  
O 4.838295 -0.063261 0.265690  
H 5.648631 0.195905 0.731383  
H 3.478941 -0.382614 1.287287  
H 3.412653 1.475654 -1.856381  
O 3.464078 0.451396 -3.342047  
H 3.988664 -0.331575 -3.045523  
H 3.906655 0.797108 -4.130968  
O 4.911347 -1.558474 -2.106114  
H 4.501963 -2.430911 -2.007519  
H 4.971134 -1.175229 -1.201132

\*\*\*\*

**TS2 0w**

C -0.399187 0.435374 -0.113299  
C -1.667796 0.818353 -0.596381  
C 0.089734 -0.978500 0.066452  
C -2.859488 -1.291697 -0.403346  
C -2.011110 -2.057395 0.524408  
O -3.861295 -2.037207 -0.753988  
N -0.611848 -1.988283 0.459583

N -2.615453 -0.146750 -1.037503  
C -2.033506 2.164211 -0.690968  
C -1.163864 3.173943 -0.288915  
H -1.449508 4.217600 -0.364239  
C 0.075398 2.807793 0.233730  
C 0.452582 1.471451 0.319334  
H 1.425441 1.223072 0.725755  
H -3.018007 2.422074 -1.073242  
O -2.506032 -2.046361 1.861016  
C 1.559006 -1.223343 -0.100899  
C 2.213243 -2.142811 0.736888  
C 2.295455 -0.605196 -1.125382  
C 3.568470 -2.420916 0.565537  
H 1.640833 -2.634848 1.516746  
C 3.649654 -0.896985 -1.307702  
C 4.292890 -1.800767 -0.459020  
H 4.061588 -3.124865 1.231356  
H 4.199606 -0.417358 -2.113529  
H 5.348422 -2.022272 -0.594764  
H -3.203439 0.082278 -1.834289  
Cl 1.183430 4.052495 0.786631  
H -2.605417 -2.961308 2.162068  
H -3.163769 -2.881414 -0.206592  
H 1.806761 0.097324 -1.795397

\*\*\*\*

**TS2 1w**

C -0.140083 0.608401 -0.174882  
C 0.890629 1.316150 -0.823280  
C -0.112460 -0.874913 -0.037604  
C 2.831133 -0.219462 -0.701360  
C 2.265621 -1.136856 0.254821  
O 4.082506 -0.077168 -0.846093  
N 0.955183 -1.564390 0.185344  
N 2.004062 0.659911 -1.413155  
C 0.816819 2.712858 -0.930051  
C -0.254128 3.424203 -0.394680  
H -0.302907 4.503927 -0.490301  
C -1.254660 2.724741 0.278919  
C -1.202237 1.339315 0.387414  
H -1.994821 0.811803 0.905861  
H 1.610374 3.251824 -1.442799  
O 3.138837 -2.245073 0.554231  
C -1.399676 -1.629490 -0.096836  
C -2.440782 -1.240478 -0.957848  
C -1.574148 -2.785437 0.684986  
C -3.619104 -1.986434 -1.036840  
H -2.323329 -0.360319 -1.583839  
C -2.754985 -3.523055 0.614460  
C -3.783576 -3.127794 -0.248236  
H -4.407366 -1.674797 -1.717606  
H -2.875339 -4.407270 1.235705  
H -4.703683 -3.703914 -0.304149  
H 2.597976 1.300615 -1.932771  
H 3.202373 -0.344162 1.411108  
Cl -2.601593 3.602140 0.992244  
O 4.293574 -0.231949 1.631315  
H 4.528514 -0.177460 0.593422  
H 4.520380 -1.152084 1.878953

H 2.701496 -3.037165 0.196221  
H -0.770810 -3.093010 1.347199

\*\*\*\*

**TS2 2w**

C -0.453180 0.607992 -0.255950  
C 0.528890 1.316791 -0.974797  
C -0.398263 -0.874998 -0.111742  
C 2.475077 -0.220570 -0.995808  
C 1.992243 -1.055389 0.070153  
O 3.678768 -0.188141 -1.386310  
N 0.694677 -1.537691 0.070641  
N 1.587863 0.648723 -1.640794  
C 0.443255 2.712180 -1.085824  
C -0.592467 3.422873 -0.483327  
H -0.653620 4.501769 -0.581427  
C -1.541415 2.722378 0.260315  
C -1.477552 1.337420 0.373482  
H -2.233081 0.810115 0.945156  
H 1.197571 3.249494 -1.656590  
O 2.935136 -2.058648 0.453035  
C -1.672847 -1.652039 -0.097981  
C -2.779013 -1.268650 -0.876627  
C -1.772931 -2.826269 0.670554  
C -3.947537 -2.034424 -0.887425  
H -2.721553 -0.375767 -1.492972  
C -2.942491 -3.584449 0.667543  
C -4.037000 -3.193008 -0.112338  
H -4.786700 -1.724468 -1.505420  
H -3.002544 -4.483252 1.276770  
H -4.948363 -3.785622 -0.115339  
H 2.104937 1.243134 -2.281345  
H 2.616000 -0.174935 1.410962  
Cl -2.841202 3.600113 1.058757  
O 3.374492 0.043033 2.133043  
H 4.675193 -0.418594 -0.271581  
H 2.779388 -2.850708 -0.092228  
O 5.235957 -0.294093 0.605513  
H 4.370498 -0.118387 1.445841  
H 3.330316 -0.704863 2.756385  
H 5.768996 0.509709 0.485491  
H -0.917839 -3.133003 1.264873

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**TS2 3w**

C -0.730677 0.587827 -0.319186  
C 0.196173 1.290215 -1.113765  
C -0.628211 -0.885319 -0.126116  
C 2.172229 -0.239911 -1.243577  
C 1.777407 -0.973603 -0.039594  
O 3.301151 -0.277260 -1.779809  
N 0.491015 -1.511573 0.012230  
N 1.236556 0.629115 -1.808362  
C 0.063399 2.677198 -1.278140  
C -0.960643 3.383650 -0.653559  
H -1.055696 4.455919 -0.789832  
C -1.853819 2.690244 0.163629  
C -1.746713 1.313890 0.327679



H -2.459527 0.790391 0.955072  
H 0.774645 3.210104 -1.905329  
O 2.722299 -2.018040 0.298833  
C -1.878056 -1.696546 -0.027533  
C -3.024146 -1.375570 -0.775479  
C -1.913886 -2.837242 0.794550  
C -4.169654 -2.172250 -0.706631  
H -3.016183 -0.508194 -1.429632  
C -3.060480 -3.626196 0.871060  
C -4.194871 -3.298269 0.119605  
H -5.041327 -1.912013 -1.302003  
H -3.071435 -4.498435 1.520310  
H -5.088319 -3.914674 0.178662  
H 1.678373 1.187053 -2.532305  
H 2.110355 0.034278 1.110424  
Cl -3.136367 3.566816 0.989844  
O 2.513983 0.683852 1.932195  
H 4.647113 -0.698005 -0.876913  
H 2.327578 -2.857302 -0.000704  
O 5.159337 -1.044236 -0.082386  
H 3.850652 0.683739 1.847735  
H 2.207329 0.307421 2.773808  
H 4.482592 -1.702178 0.224235  
O 4.952310 0.616676 1.679263  
H 5.304004 1.493182 1.454859  
H 5.123019 -0.152954 0.806066  
H -1.028881 -3.093642 1.368708

\*\*\*\*

**TS2 4w**

C 0.961456 0.555503 0.326089  
C -0.013758 1.132474 1.160916  
C 0.984202 -0.907272 0.049514  
C -1.812535 -0.602328 1.254514  
C -1.403707 -1.137787 -0.075662  
O -2.859938 -0.902933 1.872097  
N -0.073468 -1.622604 -0.115938  
N -1.004148 0.357184 1.812275  
C 0.006234 2.510656 1.413984  
C 0.966890 3.332441 0.834120  
H 0.971611 4.399562 1.029749  
C 1.912765 2.764039 -0.020245  
C 1.918078 1.396929 -0.267828  
H 2.667277 0.972236 -0.926315  
H -0.750390 2.946150 2.062154  
O -2.259198 -2.232704 -0.488827  
C 2.300759 -1.603022 -0.071239  
C 3.402104 -1.234039 0.719614  
C 2.443290 -2.680237 -0.963117  
C 4.611315 -1.927089 0.625539  
H 3.310545 -0.411865 1.423751  
C 3.653706 -3.364352 -1.064675  
C 4.743118 -2.991774 -0.269230  
H 5.449128 -1.633894 1.253090  
H 3.749630 -4.187958 -1.767904  
H 5.686434 -3.526145 -0.348310  
H -1.436758 0.788670 2.622879  
H -1.666617 -0.193567 -0.951695  
Cl 3.117080 3.789752 -0.786508

O -2.026407 0.731199 -1.809178  
H -4.060880 -1.485573 1.124699  
H -1.771723 -3.053851 -0.292172  
O -4.660989 -1.892474 0.385439  
H -3.334217 1.370743 -1.525515  
H -1.994083 0.344420 -2.698526  
H -3.911185 -2.170605 -0.226548  
O -4.265941 1.790068 -1.273615  
H -4.460601 2.459267 -1.945666  
H -5.333850 0.702826 -0.998467  
O -5.965260 -0.065790 -0.737078  
H -6.668728 0.317308 -0.191181  
H -5.227802 -1.120926 -0.078177  
H 1.593527 -2.968402 -1.574039

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**TS3 0w**

C -0.185557 -0.619921 -0.075001  
C 0.255402 -1.820896 0.545799  
C 0.702884 0.572164 -0.236085  
C 2.650904 -1.504569 0.357475  
C 2.601602 -0.702479 -0.921494  
O 3.671474 -1.797936 1.076760  
N 1.946902 0.547809 -0.577482  
N 1.578779 -2.010301 0.939323  
C -0.670418 -2.847506 0.806254  
C -1.996052 -2.736134 0.410834  
H -2.698846 -3.541082 0.600237  
C -2.414259 -1.577312 -0.253496  
C -1.533391 -0.528326 -0.476273  
H -1.886176 0.374500 -0.962432  
H -0.319937 -3.744257 1.308334  
O 3.853456 -0.489884 -1.501978  
H 4.384041 0.054719 -0.895253  
C 0.121673 1.923318 0.037688  
C -0.835935 2.123161 1.046345  
C 0.581292 3.033383 -0.691627  
C -1.319191 3.404071 1.321517  
H -1.191354 1.280469 1.632021  
C 0.086100 4.309278 -0.426099  
H 1.327850 2.879544 -1.464282  
C -0.864632 4.499255 0.582620  
H -2.050059 3.544535 2.113564  
H 0.441781 5.156740 -1.006388  
H -1.248248 5.494735 0.790890  
Cl -4.080592 -1.441840 -0.793056  
H 2.022330 -1.273071 -1.662310  
H 2.626945 -2.340456 1.725677

\*\*\*\*

**TS3 1w**

C 0.041544 0.580835 -0.206250  
C -1.169314 1.173235 0.240183  
C 0.182802 -0.894835 -0.377952  
C -2.718981 -0.616332 -0.132069  
C -1.956917 -1.061226 -1.375311  
O -3.731343 -1.311647 0.250632  
N -0.726406 -1.656002 -0.884791

N -2.324103 0.444462 0.552093  
C -1.209047 2.563894 0.459746  
C -0.110849 3.371597 0.201106  
H -0.163203 4.444065 0.358817  
C 1.066557 2.785056 -0.276297  
C 1.150869 1.412812 -0.459907  
H 2.078718 0.972627 -0.808471  
H -2.132098 3.003917 0.826247  
O -2.691157 -1.948699 -2.163312  
H -3.104980 -2.604713 -1.575163  
C 1.449421 -1.554491 0.062266  
C 2.179940 -1.088158 1.168073  
C 1.898739 -2.702823 -0.612593  
C 3.332709 -1.754905 1.589174  
H 1.838406 -0.213515 1.713909  
C 3.056104 -3.360033 -0.198314  
H 1.327143 -3.067692 -1.460036  
C 3.777009 -2.888731 0.904526  
H 3.880772 -1.388369 2.453250  
H 3.397415 -4.240733 -0.736299  
H 4.678562 -3.402800 1.227905  
H -3.194154 0.542385 1.578067  
Cl 2.456132 3.799091 -0.633528  
H -1.756402 -0.186132 -2.009556  
H -4.120926 -0.770278 1.292658  
O -4.086947 0.059012 2.181222  
H -4.877888 0.622768 2.170918

\*\*\*\*

**TS3 2w**

C 0.370664 0.563849 -0.314106  
C -0.883602 1.163307 -0.025976  
C 0.513844 -0.912493 -0.463270  
C -2.408828 -0.597226 -0.547433  
C -1.493775 -1.025611 -1.702404  
O -3.447958 -1.315263 -0.355463  
N -0.342626 -1.654272 -1.078031  
N -2.073819 0.446923 0.190181  
C -0.943777 2.560896 0.150869  
C 0.180971 3.361638 0.007964  
H 0.112482 4.438086 0.128838  
C 1.406043 2.763314 -0.306241  
C 1.506358 1.387523 -0.450287  
H 2.466782 0.938494 -0.679187  
H -1.903399 3.011065 0.388817  
O -2.140753 -1.888111 -2.589245  
H -2.742634 -2.445531 -2.063394  
C 1.708276 -1.591898 0.124093  
C 2.324123 -1.120897 1.295704  
C 2.203932 -2.761378 -0.478304  
C 3.409048 -1.802413 1.852102  
H 1.946464 -0.227819 1.785128  
C 3.293696 -3.434415 0.071901  
H 1.719840 -3.129594 -1.377260  
C 3.900310 -2.957730 1.239504  
H 3.868627 -1.429695 2.763954  
H 3.672102 -4.331752 -0.411108  
H 4.749825 -3.483740 1.667724  
H -2.890559 0.874554 1.243974

Cl 2.834102 3.768131 -0.512726  
H -1.198081 -0.142577 -2.286320  
O -3.642711 1.128321 2.052421  
H -4.458843 0.160631 1.860744  
O -4.988391 -0.781848 1.460959  
H -5.864178 -0.560900 1.103806  
H -4.295569 -1.066773 0.610979  
H -3.212670 1.065173 2.920514

\*\*\*\*

**TS3 3w**

C -0.616684 0.541234 -0.329602  
C 0.699305 1.071804 -0.181960  
C -0.863464 -0.902622 -0.599485  
C 2.044145 -0.731487 -1.031351  
C 0.984755 -1.093349 -2.088884  
O 3.066185 -1.478683 -0.967534  
N -0.146767 -1.651951 -1.367539  
N 1.879892 0.333419 -0.247325  
C 0.825866 2.446939 0.133805  
C -0.273520 3.281940 0.251876  
H -0.143496 4.335537 0.478772  
C -1.556756 2.752337 0.069579  
C -1.726949 1.404664 -0.197914  
H -2.727039 1.004137 -0.322483  
H 1.822248 2.850857 0.283052  
O 0.694157 -0.042116 -2.999714  
H 0.271871 0.697149 -2.533158  
C -2.023738 -1.565382 0.075003  
C -2.704009 -2.604242 -0.582770  
C -2.416638 -1.218620 1.378662  
C -3.757117 -3.270462 0.042887  
H -2.392049 -2.877873 -1.585541  
C -3.461860 -1.896370 2.010166  
H -1.893066 -0.428663 1.909374  
C -4.139031 -2.920030 1.342367  
H -4.281109 -4.064387 -0.483412  
H -3.745623 -1.623782 3.023508  
H -4.958915 -3.441234 1.830259  
H 3.103267 0.954800 0.290317  
Cl -2.959589 3.807259 0.191381  
H 1.405907 -1.880287 -2.712944  
O 3.996793 1.449207 0.679779  
H 4.680768 0.615749 1.484594  
O 5.183420 -0.162201 2.092856  
H 4.906900 -0.068681 3.019359  
H 4.803070 -1.179897 1.646521  
O 4.307055 -2.171366 1.077774  
H 4.975581 -2.799164 0.759486  
H 3.753251 -1.840885 0.227686  
H 4.532868 1.716096 -0.084399

\*\*\*\*

**TS3 4w**

C 1.026536 0.589000 -0.452909  
C -0.133291 1.409186 -0.426611  
C 0.943762 -0.866955 -0.756883  
C -1.722007 0.051927 -1.538572

C -0.621874 -0.456721 -2.475874  
O -2.884092 -0.484334 -1.717068  
N 0.177070 -1.362485 -1.668059  
N -1.444344 0.938811 -0.614152  
C 0.010005 2.772580 -0.095744  
C 1.252885 3.334275 0.160016  
H 1.344947 4.390130 0.393562  
C 2.390786 2.521316 0.107087  
C 2.281832 1.168518 -0.177321  
H 3.172334 0.549797 -0.201604  
H -0.882206 3.391385 -0.059239  
O -1.130813 -1.084215 -3.614730  
H -1.908121 -1.603818 -3.343331  
C 1.781947 -1.826549 0.024125  
C 2.113786 -1.592689 1.369163  
C 2.210991 -3.020547 -0.581248  
C 2.854536 -2.530669 2.092292  
H 1.781269 -0.681623 1.858318  
C 2.959027 -3.951022 0.138405  
H 1.946466 -3.203406 -1.617878  
C 3.283056 -3.710086 1.478307  
H 3.096581 -2.338164 3.134428  
H 3.292186 -4.865114 -0.346474  
H 3.866616 -4.436274 2.038496  
H -2.533236 1.476077 0.388554  
Cl 3.973371 3.223757 0.412202  
H -0.025024 0.392847 -2.835381  
O -3.380216 1.719288 0.967166  
H -4.131928 1.062570 0.464482  
O -4.714403 0.067023 -0.215465  
H -5.505130 0.339935 -0.706520  
H -3.771532 -0.211554 -1.008007  
H -3.261407 1.335046 1.888422  
O -3.370783 0.403889 3.288247  
H -3.878846 -0.398160 3.001135  
H -2.583932 0.092205 3.758335  
O -4.880570 -1.494612 2.035037  
H -4.680117 -2.430181 1.886520  
H -4.920161 -1.065531 1.143340

\*\*\*\*

## XYZ coordinates for Table S4

**Cat1' 0w (fixed C3-O bond)**

C -0.173499 -0.615590 -0.002662  
 C 0.404577 -1.776508 0.568671  
 C 0.567025 0.663104 -0.184828  
 C 2.833625 -1.309698 0.415098  
 C 2.516696 -0.473747 -0.837944  
 O 4.000453 -1.415842 0.782557  
 N 1.811956 0.707564 -0.559772  
 N 1.750146 -1.823210 1.031262  
 C -0.372399 -2.927227 0.753870  
 C -1.702059 -2.965303 0.350826  
 H -2.291675 -3.865279 0.490847  
 C -2.267703 -1.837694 -0.254349  
 C -1.518834 -0.677050 -0.417245  
 H -1.974788 0.193095 -0.875327  
 H 0.074244 -3.807129 1.209466  
 O 3.872497 -0.006601 -1.257524  
 C -0.121512 1.948993 0.049042  
 C -1.111133 2.068871 1.044587  
 C 0.246525 3.087785 -0.693721  
 C -1.710275 3.302710 1.294461  
 H -1.392475 1.207822 1.643116  
 C -0.369328 4.312761 -0.453801  
 H 0.998694 2.998359 -1.471027  
 C -1.346114 4.423675 0.543012  
 H -2.460267 3.388567 2.075146  
 H -0.093487 5.181084 -1.045002  
 H -1.822949 5.381402 0.731203  
 H 2.153555 -1.072828 -1.681329  
 Cl -3.920747 -1.881885 -0.797108  
 H 1.955434 -2.424783 1.825620  
 H 4.491136 -0.331969 -0.690583  
 H 3.843410 0.982269 -1.212091

\*\*\*\*

**Cat1' 1w (fixed C3-O bond)**

C 0.707237 -0.513653 -0.019359  
 C 0.734614 -1.819457 -0.567890  
 C -0.526609 0.308970 0.062462  
 C -1.662638 -2.472253 -0.548716  
 C -1.847226 -1.543245 0.664447  
 O -2.609051 -3.128840 -0.966783  
 N -1.701980 -0.170836 0.337912  
 N -0.419535 -2.461344 -1.086702  
 C 1.951875 -2.506343 -0.674849  
 C 3.135823 -1.940928 -0.217684  
 H 4.070274 -2.486390 -0.297824  
 C 3.109795 -0.667098 0.361756  
 C 1.916981 0.040748 0.447034  
 H 1.914496 1.033617 0.881952  
 H 1.968063 -3.501194 -1.112242  
 O -3.271196 -1.759437 1.054735  
 C -0.436011 1.771297 -0.171345  
 C 0.367376 2.287743 -1.204073  
 C -1.190940 2.656519 0.620765  
 C 0.392959 3.659985 -1.453884  
 H 0.951735 1.616836 -1.827115

C -1.144040 4.029172 0.382279  
 H -1.775280 2.268387 1.450883  
 C -0.358580 4.532175 -0.660862  
 H 1.002144 4.048072 -2.264947  
 H -1.709310 4.707441 1.015070  
 H -0.325298 5.601592 -0.848479  
 H -1.258323 -1.868514 1.530337  
 Cl 4.581446 0.041191 0.966872  
 H -0.282181 -3.135012 -1.836128  
 H -3.629273 -2.407723 0.542846  
 H -3.857280 -0.822424 0.978508  
 O -4.386912 0.421925 0.871119  
 H -5.215337 0.566945 0.381350  
 H -3.654838 0.892427 0.417440

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**Cat1' 2w (fixed C3-O bond)**

C -0.745246 -0.623206 0.078555  
 C -0.097104 -1.670149 0.776221  
 C -0.113807 0.709022 -0.130264  
 C 2.284822 -0.943142 0.756023  
 C 1.960248 -0.271388 -0.591736  
 O 3.406363 -0.910739 1.247910  
 N 1.140440 0.856560 -0.424151  
 N 1.202207 -1.525943 1.333156  
 C -0.762274 -2.885387 0.991462  
 C -2.043990 -3.094619 0.497122  
 H -2.548000 -4.041192 0.661832  
 C -2.672288 -2.078431 -0.231754  
 C -2.038546 -0.856625 -0.428024  
 H -2.544101 -0.072388 -0.980052  
 H -0.264199 -3.678030 1.543721  
 O 3.248024 0.241818 -1.144230  
 C -0.937310 1.935141 -0.012355  
 C -2.016114 2.004484 0.888996  
 C -0.610694 3.069708 -0.779047  
 C -2.746163 3.185526 1.023843  
 H -2.270931 1.146575 1.503948  
 C -1.353530 4.240871 -0.653965  
 H 0.216765 3.016392 -1.479373  
 C -2.421035 4.302527 0.249479  
 H -3.568215 3.232475 1.732170  
 H -1.105553 5.105187 -1.263484  
 H -2.998348 5.217661 0.347050  
 H 1.629161 -0.998888 -1.344288  
 Cl -4.265552 -2.341555 -0.887897  
 H 1.405225 -2.035125 2.189364  
 H 3.832134 -0.438142 -1.228675  
 H 3.587228 0.897662 -0.629708  
 O 4.496246 1.899277 0.391390  
 H 4.584337 1.565083 1.299150  
 H 4.442991 2.866216 0.447953  
 O 4.738420 -1.874838 -1.282259  
 H 5.111924 -2.118361 -0.418708  
 H 5.371196 -2.163134 -1.959514

\*\*\*\*

**Cat1' 3w (fixed C3-O bond)**

C 1.280353 -0.438834 -0.078611  
 C 1.086250 -1.657530 -0.770519  
 C 0.184405 0.549467 0.117761  
 C -1.393601 -1.912717 -0.753878  
 C -1.363739 -1.144841 0.581661  
 O -2.429646 -2.346766 -1.239402  
 N -1.031913 0.208652 0.404380  
 N -0.165891 -2.027381 -1.328709  
 C 2.168541 -2.525088 -0.976920  
 C 3.430323 -2.224032 -0.479000  
 H 4.259808 -2.905404 -0.636676  
 C 3.616829 -1.041113 0.245173  
 C 2.562017 -0.155439 0.432394  
 H 2.725418 0.765534 0.980591  
 H 2.015323 -3.451092 -1.525096  
 O -2.752431 -1.155000 1.131380  
 C 0.476970 1.998241 -0.003840  
 C 1.453488 2.472512 -0.899034  
 C -0.262983 2.923464 0.755973  
 C 1.680621 3.842494 -1.033499  
 H 2.020309 1.775653 -1.509136  
 C -0.020222 4.289278 0.631773  
 H -1.014189 2.558906 1.449364  
 C 0.950219 4.752338 -0.264525  
 H 2.428147 4.197885 -1.736836  
 H -0.581927 4.994579 1.237880  
 H 1.137680 5.818216 -0.360335  
 H -0.781301 -1.682005 1.341927  
 Cl 5.186770 -0.669379 0.907439  
 H -0.152035 -2.597441 -2.170228  
 H -3.040911 -2.004708 1.201170  
 H -3.308679 -0.665662 0.619604  
 O -4.560181 -0.066054 -0.279630  
 H -4.625398 -0.335390 -1.208324  
 H -4.986532 0.818474 -0.199945  
 O -3.332131 -3.686334 1.212972  
 H -3.548343 -3.987373 0.314193  
 H -3.875177 -4.203184 1.829110  
 O -5.829694 2.373264 -0.012360  
 H -5.562753 3.241170 -0.352431  
 H -6.764064 2.450297 0.235885

\*\*\*\*

**Cat1' 4w (fixed C3-O bond)**

C 1.356737 -0.638619 -0.217364  
 C 0.832734 -1.555130 -1.159635  
 C 0.657334 0.627070 0.137822  
 C -1.564869 -0.881550 -1.302184  
 C -1.424843 -0.440765 0.167414  
 O -2.617496 -0.800922 -1.918060  
 N -0.625207 0.709029 0.294399  
 N -0.395383 -1.335401 -1.834544  
 C 1.564422 -2.702209 -1.500672  
 C 2.787041 -2.975010 -0.899762  
 H 3.341907 -3.868851 -1.164935  
 C 3.287442 -2.094297 0.065714  
 C 2.590312 -0.937590 0.393638  
 H 2.999570 -0.254826 1.129658  
 H 1.163293 -3.392468 -2.238293

O -2.783306 -0.059238 0.652928  
C 1.448919 1.866145 0.340578  
C 2.620654 2.114145 -0.397407  
C 0.998541 2.834975 1.256407  
C 3.322091 3.308171 -0.226295  
H 2.973820 1.386784 -1.122316  
C 1.711866 4.017533 1.437526  
H 0.097000 2.642625 1.829359  
C 2.873638 4.258428 0.694901  
H 4.218350 3.494538 -0.810988  
H 1.367288 4.750253 2.161979  
H 3.428361 5.181819 0.836658  
H -1.150203 -1.283946 0.814245  
Cl 4.803729 -2.444695 0.854910  
H -0.484027 -1.705064 -2.777095  
H -3.323885 -0.779527 0.634210  
H -3.129410 0.615667 0.168483  
O -4.002293 1.650762 -0.778088  
H -3.961104 1.389528 -1.711426  
H -4.028760 2.633994 -0.752056  
O -4.052794 -2.272531 0.543241  
H -4.445023 -2.481753 -0.318880  
H -4.648709 -2.653337 1.230374  
O -4.171477 4.416229 -0.806413  
H -3.467269 5.076368 -0.715629  
H -5.010217 4.891041 -0.699492  
O -5.707715 -3.346196 2.472937  
H -5.601961 -4.220080 2.879913  
H -6.549730 -2.990968 2.797328

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**Cat1 0w**

C -0.163554 -0.607742 -0.019654  
C 0.405342 -1.755755 0.576909  
C 0.580383 0.676166 -0.206880  
C 2.769764 -1.225765 0.387234  
C 2.543126 -0.463661 -0.905834  
O 3.962106 -1.285497 0.890384  
N 1.819003 0.736120 -0.585615  
N 1.766050 -1.779161 1.022451  
C -0.352424 -2.910113 0.797828  
C -1.679203 -2.965793 0.387413  
H -2.265472 -3.864868 0.544598  
C -2.245577 -1.853988 -0.247199  
C -1.505210 -0.688056 -0.432894  
H -1.967836 0.170244 -0.906442  
H 0.100190 -3.774826 1.276330  
O 3.832392 -0.144247 -1.383477  
C -0.124059 1.955304 0.039430  
C -1.124567 2.061105 1.025115  
C 0.247705 3.103291 -0.686661  
C -1.733164 3.289499 1.280842  
H -1.410701 1.193936 1.612956  
C -0.376338 4.323039 -0.440267  
H 1.014723 3.024517 -1.450056  
C -1.365603 4.419797 0.545401  
H -2.492790 3.363710 2.053461  
H -0.095194 5.198934 -1.017657  
H -1.848811 5.373437 0.738123

H 2.025873 -1.114578 -1.628932  
Cl -3.892660 -1.921069 -0.795688  
H 1.980968 -2.296530 1.874778  
H 4.564016 -0.842094 0.233837  
H 3.859168 0.821568 -1.522110

\*\*\*\*

**Cat1 1w**

C -0.716118 -0.509939 0.020903  
C -0.753208 -1.813732 0.572385  
C 0.524014 0.309070 -0.062139  
C 1.633735 -2.456458 0.557952  
C 1.831695 -1.548846 -0.668731  
O 2.607180 -3.081701 0.985844  
N 1.695147 -0.173809 -0.344676  
N 0.400537 -2.460784 1.094453  
C -1.970988 -2.497957 0.677308  
C -3.151512 -1.930019 0.213193  
H -4.088154 -2.472089 0.290491  
C -3.117656 -0.658323 -0.369579  
C -1.921630 0.046140 -0.451773  
H -1.914552 1.037937 -0.889125  
H -1.991458 -3.491553 1.117386  
O 3.245357 -1.808320 -1.018669  
C 0.438162 1.771043 0.175524  
C -0.380720 2.291998 1.193759  
C 1.214732 2.652214 -0.600101  
C -0.402450 3.664207 1.444528  
H -0.981016 1.625136 1.805910  
C 1.172706 4.024617 -0.360623  
H 1.814927 2.258939 -1.416055  
C 0.369944 4.532134 0.667209  
H -1.024484 4.055403 2.244268  
H 1.755435 4.699801 -0.980792  
H 0.340118 5.601582 0.855295  
H 1.241663 -1.877114 -1.532641  
Cl -4.583500 0.053316 -0.983584  
H 0.268467 -3.110180 1.866147  
H 3.534096 -2.454886 -0.283187  
H 3.824928 -0.912903 -0.978259  
O 4.474198 0.373620 -0.926423  
H 5.374592 0.509642 -0.585930  
H 3.857036 0.940383 -0.425932

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**Cat1 2w**

C -0.732226 -0.634844 0.064270  
C -0.078924 -1.682577 0.755708  
C -0.106062 0.701554 -0.136591  
C 2.292365 -0.932636 0.731349  
C 1.971589 -0.273142 -0.622136  
O 3.410388 -0.873389 1.240034  
N 1.145948 0.860164 -0.431937  
N 1.221860 -1.533848 1.308033  
C -0.738996 -2.900571 0.970078  
C -2.022324 -3.111713 0.480605  
H -2.523029 -4.060286 0.643805  
C -2.656626 -2.094351 -0.241531

C -2.027397 -0.869930 -0.436332  
H -2.538312 -0.084726 -0.982036  
H -0.235970 -3.693643 1.517253  
O 3.229303 0.229112 -1.196645  
C -0.937769 1.922479 -0.005895  
C -2.002535 1.985348 0.911979  
C -0.633627 3.057170 -0.781304  
C -2.739905 3.160975 1.056014  
H -2.241866 1.125919 1.531197  
C -1.383834 4.223010 -0.646984  
H 0.180247 3.006670 -1.497749  
C -2.436352 4.278809 0.274117  
H -3.551227 3.202801 1.776958  
H -1.154097 5.087078 -1.264039  
H -3.019637 5.189389 0.378542  
H 1.598709 -1.005584 -1.350415  
Cl -4.252415 -2.359483 -0.891094  
H 1.426741 -2.030150 2.171379  
H 3.933201 -0.521737 -1.250005  
H 3.620268 0.982809 -0.581110  
O 4.298936 1.902535 0.384663  
H 4.304149 1.470352 1.257587  
H 3.899372 2.781177 0.498582  
O 4.884590 -1.739055 -1.182909  
H 5.177601 -1.891376 -0.267484  
H 5.650254 -1.862811 -1.767781

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**Cat1 3w**

C -0.932945 -0.608353 0.148766  
C -0.472385 -1.675750 0.958438  
C -0.103475 0.593881 -0.131134  
C 1.976029 -1.248418 0.996167  
C 1.818879 -0.747009 -0.455284  
O 3.038088 -1.238564 1.630160  
N 1.171779 0.544658 -0.369184  
N 0.813981 -1.671439 1.554534  
C -1.325762 -2.747802 1.255452  
C -2.614181 -2.797906 0.737852  
H -3.265003 -3.635630 0.965581  
C -3.061003 -1.764407 -0.094295  
C -2.239314 -0.678796 -0.373492  
H -2.605970 0.124098 -1.003175  
H -0.969463 -3.554458 1.890676  
O 3.066570 -0.584774 -1.101382  
C -0.749607 1.930915 -0.142031  
C -1.758309 2.260593 0.781047  
C -0.323317 2.901200 -1.068354  
C -2.313767 3.540374 0.788776  
H -2.093113 1.526116 1.507809  
C -0.894464 4.172892 -1.069239  
H 0.432020 2.639000 -1.803898  
C -1.886652 4.496563 -0.137140  
H -3.081186 3.789764 1.515816  
H -0.575992 4.907958 -1.803166  
H -2.330404 5.488148 -0.137780  
H 1.218186 -1.473525 -1.020922  
Cl -4.664747 -1.833316 -0.774856  
H 0.904645 -2.059959 2.489953

H 3.284695 -1.392545 -1.631582  
H 4.271331 0.148258 -0.253400  
O 4.655241 0.535752 0.602061  
H 4.247811 -0.122981 1.252285  
H 4.120851 1.428574 0.710834  
O 3.504139 -2.839410 -2.547090  
H 4.130642 -3.533221 -2.284817  
H 3.522111 -2.811217 -3.517402  
O 2.999187 2.435264 0.697335  
H 2.254748 2.006488 0.197047  
H 3.110308 3.344971 0.379406

\*\*\*\*

**Cat1 4w**

C 1.033720 -0.678590 -0.337119  
C 0.491055 -1.426297 -1.410859  
C 0.493218 0.648423 0.061445  
C -1.716713 -0.323633 -1.719171  
C -1.730798 -0.123483 -0.188012  
O -2.595981 0.082109 -2.486903  
N -0.773626 0.926666 0.092669  
N -0.607810 -0.962309 -2.175390  
C 1.091078 -2.633926 -1.795746  
C 2.196698 -3.129636 -1.116018  
H 2.649315 -4.069199 -1.415300  
C 2.712863 -2.413171 -0.029675  
C 2.150186 -1.199392 0.345961  
H 2.573288 -0.645425 1.176427  
H 0.677459 -3.193483 -2.630594  
O -2.997986 0.279623 0.286805  
C 1.439475 1.727175 0.446485  
C 2.659261 1.903383 -0.230791  
C 1.097085 2.613547 1.484649  
C 3.508285 2.956432 0.111173  
H 2.935027 1.232749 -1.039496  
C 1.957026 3.653271 1.835542  
H 0.170560 2.459937 2.030795  
C 3.161517 3.830084 1.145788  
H 4.440893 3.093055 -0.428608  
H 1.695048 4.318689 2.653509  
H 3.830474 4.641325 1.418919  
H -1.458717 -1.071408 0.297542  
Cl 4.080931 -3.042613 0.850925  
H -0.609170 -1.161243 -3.172510  
H -3.528066 -0.523451 0.567706  
H -3.743262 1.398784 -0.543481  
O -3.894112 2.046725 -1.325763  
H -3.565718 1.450125 -2.066470  
H -3.154765 2.764653 -1.172059  
O -4.238133 -1.943033 0.998298  
H -4.961370 -2.311314 0.468146  
H -4.467967 -2.109791 1.943066  
O -1.831437 3.408142 -0.786004  
H -1.328869 2.704350 -0.295386  
H -1.773739 4.238480 -0.288120  
O -4.845128 -2.429195 3.648360  
H -4.627365 -3.252638 4.112240  
H -5.500350 -1.970358 4.196738

\*\*\*\*

**Cat2 0w**

C -0.529277 -0.329500 -0.011726  
C -0.868099 -1.561839 0.589937  
C 0.885356 0.109070 -0.213000  
C 1.263082 -2.733472 0.410130  
C 1.503176 -2.069257 -0.940802  
O 2.208159 -3.494839 0.884312  
N 1.820601 -0.696822 -0.607894  
N 0.143483 -2.470856 1.053877  
C -2.200647 -1.922807 0.812951  
C -3.227914 -1.081797 0.402175  
H -4.263905 -1.363282 0.557776  
C -2.911365 0.126468 -0.231674  
C -1.583514 0.504225 -0.422282  
H -1.357505 1.450426 -0.900641  
H -2.438291 -2.869906 1.290831  
O 2.524800 -2.678547 -1.646632  
C 1.245464 1.523682 0.035507  
C 0.578066 2.291551 1.009428  
C 2.308789 2.101964 -0.684431  
C 0.970121 3.606448 1.259175  
H -0.230348 1.859061 1.591826  
C 2.684903 3.420392 -0.442746  
H 2.821420 1.513024 -1.437882  
C 2.018638 4.174670 0.530350  
H 0.457792 4.186102 2.021494  
H 3.495039 3.863160 -1.014839  
H 2.315510 5.202630 0.718230  
H 0.578190 -2.178764 -1.528911  
Cl -4.187296 1.171108 -0.776772  
H 3.353948 -2.200471 -1.463815  
H -0.050902 -2.942206 1.936534  
H 2.070130 -3.826559 1.793244

\*\*\*\*

**Cat2 1w**

C 0.153429 -0.597497 0.204369  
C -1.026865 -1.263999 -0.192255  
C 0.216194 0.883842 0.393985  
C -2.691572 0.454910 0.292519  
C -1.883058 0.881368 1.510929  
O -3.762274 1.117169 -0.006943  
N -0.727808 1.561814 0.964116  
N -2.244233 -0.550469 -0.440842  
C -1.038392 -2.645366 -0.413259  
C 0.111902 -3.397436 -0.206700  
H 0.102875 -4.470891 -0.362911  
C 1.279666 -2.756050 0.223863  
C 1.305146 -1.376433 0.413085  
H 2.222627 -0.894689 0.731704  
H -1.954330 -3.136912 -0.730910  
O -2.607377 1.700899 2.361055  
C 1.411131 1.623064 -0.080921  
C 2.141203 1.197108 -1.206616  
C 1.797310 2.805010 0.579177  
C 3.229970 1.940502 -1.663060  
H 1.848914 0.298663 -1.742492

C 2.894283 3.535066 0.129131  
H 1.237768 3.132792 1.449149  
C 3.611670 3.106479 -0.993746  
H 3.779123 1.609051 -2.539644  
H 3.194056 4.436822 0.655269  
H 4.466391 3.678468 -1.343793  
H -1.626529 -0.030208 2.073336  
Cl 2.717395 -3.690493 0.515065  
H -2.448717 2.626904 2.104229  
H -2.808665 -0.848940 -1.238120  
H -4.198445 0.806964 -0.852556  
O -4.649074 -0.048367 -2.256851  
H -5.522366 -0.478120 -2.238873  
H -4.606427 0.428052 -3.104522

\*\*\*\*

**Cat2 2w**

C 0.391476 0.553824 -0.347305  
C -0.874765 1.141426 -0.133404  
C 0.578292 -0.924837 -0.460563  
C -2.345536 -0.710340 -0.725757  
C -1.358964 -1.099795 -1.823978  
O -3.376125 -1.455722 -0.547223  
N -0.237230 -1.684218 -1.117214  
N -2.060152 0.349832 0.017158  
C -1.009841 2.528500 -0.005037  
C 0.100093 3.357519 -0.118997  
H -0.005741 4.434231 -0.038292  
C 1.355655 2.788668 -0.362312  
C 1.502630 1.407741 -0.463101  
H 2.484031 0.983085 -0.642354  
H -1.992225 2.961523 0.161232  
O -1.906674 -1.983433 -2.739471  
C 1.751671 -1.558972 0.189771  
C 2.313281 -1.033170 1.368229  
C 2.291798 -2.737523 -0.358520  
C 3.388503 -1.673830 1.984826  
H 1.901679 -0.134250 1.818258  
C 3.374226 -3.365706 0.252353  
H 1.861661 -3.142974 -1.268460  
C 3.924376 -2.837052 1.425768  
H 3.807742 -1.264145 2.899381  
H 3.793302 -4.265874 -0.188119  
H 4.768723 -3.329110 1.900385  
H -1.095525 -0.186953 -2.379407  
Cl 2.748459 3.818281 -0.536180  
H -1.789112 -2.889995 -2.404288  
H -2.710720 0.651429 0.751064  
H -3.996296 -1.228873 0.231667  
O -5.027759 -0.914879 1.365916  
H -5.582468 -1.611215 1.751897  
H -4.766608 -0.283722 2.066437  
O -3.707550 1.269779 2.417893  
H -4.267408 2.065003 2.398304  
H -3.205652 1.327105 3.248984

\*\*\*\*

**Cat2 3w**

C -0.970016 0.524984 0.343736  
C 0.130223 1.399156 0.202575  
C -0.798315 -0.946122 0.543072  
C 1.945349 0.006735 1.056756  
C 0.969110 -0.566456 2.082855  
O 3.137068 -0.453163 1.026040  
N 0.105454 -1.445511 1.320923  
N 1.481279 0.924980 0.215290  
C -0.067015 2.768046 -0.013421  
C -1.351752 3.296825 -0.061467  
H -1.504729 4.360264 -0.211947  
C -2.448082 2.443970 0.109709  
C -2.262450 1.077329 0.298039  
H -3.123121 0.429112 0.418932  
H 0.791672 3.424600 -0.122040  
O 1.611369 -1.240836 3.109735  
C -1.703278 -1.885699 -0.166678  
C -2.253632 -1.571409 -1.422953  
C -1.983826 -3.139402 0.408152  
C -3.062756 -2.492207 -2.089930  
H -2.037408 -0.615963 -1.892231  
C -2.802675 -4.050251 -0.254779  
H -1.562347 -3.381589 1.378268  
C -3.342848 -3.730278 -1.505708  
H -3.474536 -2.242038 -3.063555  
H -3.024903 -5.008994 0.205109  
H -3.981539 -4.442402 -2.020830  
H 0.431439 0.274377 2.545912  
Cl -4.062089 3.099075 0.081891  
H 1.793529 -2.150822 2.816039  
H 2.108216 1.338280 -0.483683  
H 3.801616 -0.087146 0.293725  
O 4.794582 0.418853 -0.639330  
H 5.581031 -0.142560 -0.859995  
H 4.450735 0.831341 -1.454331  
O 3.048003 2.008469 -2.136319  
H 3.399657 2.913320 -2.190543  
H 2.636104 1.837795 -3.000242  
O 7.002759 -1.038949 -1.282229  
H 7.872834 -0.737804 -0.975479  
H 7.051646 -2.006649 -1.331688

\*\*\*\*

**Cat2 4w**

C 1.497706 -0.620329 -0.002726  
C 0.583495 -1.528620 -0.582152  
C 1.109031 0.771620 0.364851  
C -1.599901 -0.459459 -0.063847  
C -0.965741 0.035072 1.247533  
O -2.769619 -0.205231 -0.370502  
N -0.022359 1.067117 0.914955  
N -0.764459 -1.171248 -0.859176  
C 1.007388 -2.809845 -0.961214  
C 2.317641 -3.219090 -0.743996  
H 2.637835 -4.215042 -1.031440  
C 3.216381 -2.337758 -0.133116  
C 2.817912 -1.053622 0.221300  
H 3.530918 -0.376054 0.677360  
H 0.299210 -3.495818 -1.418987

O -1.944692 0.569766 2.113347  
C 2.060487 1.882324 0.100727  
C 2.921029 1.858350 -1.011571  
C 2.075248 3.002242 0.951761  
C 3.771743 2.934114 -1.269535  
H 2.913394 1.010246 -1.690090  
C 2.937597 4.067141 0.700402  
H 1.414782 3.020738 1.812727  
C 3.786479 4.037046 -0.411763  
H 4.423070 2.909235 -2.138608  
H 2.952201 4.919697 1.373673  
H 4.457798 4.868795 -0.606749  
H -0.512655 -0.821335 1.769104  
Cl 4.855332 -2.851055 0.176505  
H -1.951324 1.532825 1.963236  
H -1.186396 -1.565985 -1.694757  
H -4.173515 -0.415815 -1.134618  
O -5.147747 -0.516862 -1.367385  
H -5.689572 -0.579791 -0.436442  
H -5.456664 0.277022 -1.903877  
O -5.946334 1.534074 -2.839233  
H -6.383467 1.390535 -3.693946  
H -6.295370 2.365782 -2.480797  
O -6.324093 -0.610017 0.815963  
H -6.885730 -1.386598 0.971684  
H -5.652511 -0.569989 1.563885  
O -4.435007 -0.576752 2.672916  
H -3.563354 -0.173703 2.451588  
H -4.590605 -0.412833 3.615234

\*\*\*\*

**Cat3 0w**

C 0.123670 -0.620964 -0.007972  
C 1.174010 -1.420585 0.531041  
C 0.199567 0.832977 -0.131015  
C 3.195879 0.040210 0.387283  
C 2.592572 0.722980 -0.855261  
O 4.299446 0.360686 0.786114  
N 1.349898 1.405697 -0.428119  
N 2.399327 -0.897947 0.990835  
C 0.958336 -2.796349 0.703543  
C -0.234202 -3.396102 0.321787  
H -0.372686 -4.464654 0.451481  
C -1.252186 -2.620223 -0.251546  
C -1.080782 -1.253048 -0.401510  
H -1.873213 -0.660269 -0.843232  
H 1.748972 -3.406599 1.131554  
O 3.452063 1.671847 -1.357159  
C -0.967533 1.698168 0.065218  
C -1.913198 1.401819 1.070182  
C -1.126715 2.863802 -0.716898  
C -2.982000 2.265008 1.296250  
H -1.789073 0.520742 1.691758  
C -2.209300 3.709423 -0.496035  
H -0.438969 3.077961 -1.531447  
C -3.133317 3.415210 0.514162  
H -3.695787 2.042742 2.083596  
H -2.340739 4.590462 -1.116737  
H -3.974700 4.079972 0.687033

H 2.319578 -0.017235 -1.620056  
Cl -2.732438 -3.372670 -0.766577  
H 4.245551 1.693297 -0.778235  
H 2.866358 -1.411452 1.734627  
H 1.430696 2.421944 -0.404562

\*\*\*\*

**Cat3 1w**

C 0.103703 -0.442853 -0.219593  
C 1.484258 -0.596153 0.110332  
C -0.585417 0.842161 -0.214544  
C 2.440774 1.684006 -0.137261  
C 1.389601 1.996865 -1.220861  
O 3.283723 2.521773 0.140663  
N 0.055965 1.933597 -0.584471  
N 2.340729 0.461217 0.459853  
C 2.019385 -1.894030 0.190394  
C 1.250016 -3.012580 -0.094344  
H 1.690059 -4.003520 -0.043830  
C -0.094781 -2.860706 -0.466545  
C -0.662350 -1.599153 -0.512979  
H -1.702421 -1.490414 -0.797406  
H 3.061594 -2.012201 0.472095  
O 1.566131 3.267870 -1.718335  
C -1.988735 0.979997 0.193600  
C -2.490827 0.232953 1.279721  
C -2.833522 1.897182 -0.468766  
C -3.805045 0.416121 1.702156  
H -1.843736 -0.460216 1.807847  
C -4.151592 2.058394 -0.051547  
H -2.477957 2.440861 -1.340718  
C -4.636241 1.324136 1.037319  
H -4.181212 -0.147682 2.550393  
H -4.804154 2.746571 -0.580187  
H -5.663960 1.455751 1.363268  
H 1.411801 1.243977 -2.021031  
Cl -1.049944 -4.261091 -0.861710  
H 2.326584 3.664977 -1.238233  
H 3.137376 0.221823 1.072317  
H -0.387035 2.844972 -0.472596  
O 4.622548 -0.364985 1.986843  
H 4.657753 -0.509249 2.946193  
H 5.432924 0.123900 1.767420

\*\*\*\*

**Cat3 2w**

C 0.236110 0.395701 -0.473477  
C -1.191922 0.440228 -0.458904  
C 1.003933 -0.822586 -0.255124  
C -1.889853 -1.917775 -0.793321  
C -0.603725 -2.176450 -1.603851  
O -2.701294 -2.821055 -0.661092  
N 0.545930 -1.978154 -0.696109  
N -2.025744 -0.670408 -0.261119  
C -1.827746 1.693021 -0.547203  
C -1.101484 2.862870 -0.707355  
H -1.615355 3.815128 -0.792322  
C 0.300119 2.814471 -0.775746

C 0.958007 1.605270 -0.643691  
H 2.040253 1.576572 -0.690980  
H -2.911585 1.728913 -0.491546  
O -0.570292 -3.474860 -2.060192  
C 2.291579 -0.826710 0.452276  
C 2.487670 -0.004082 1.580796  
C 3.326988 -1.690492 0.034448  
C 3.688807 -0.060239 2.283444  
H 1.690888 0.649690 1.921085  
C 4.530972 -1.725948 0.732407  
H 3.211698 -2.291910 -0.864093  
C 4.710773 -0.916732 1.860226  
H 3.827722 0.562505 3.161989  
H 5.332507 -2.374420 0.391857  
H 5.649844 -0.949738 2.405076  
H -0.503851 -1.456330 -2.427799  
Cl 1.209172 4.280603 -1.017392  
H -1.386945 -3.914376 -1.732662  
H -2.968903 -0.467899 0.130374  
H 1.020894 -2.843202 -0.441085  
O -4.564456 0.117647 0.626355  
H -4.792776 0.177504 1.583051  
H -5.310323 -0.335707 0.203168  
O -5.161045 0.330083 3.336092  
H -5.352311 -0.421886 3.918305  
H -5.673670 1.077036 3.683009

\*\*\*\*

**Cat3 3w**

C -0.669879 -0.274599 -0.618146  
C 0.702170 0.049444 -0.852460  
C -1.631416 0.664626 -0.059512  
C 0.764494 2.528096 -0.863722  
C -0.685587 2.555004 -1.388734  
O 1.358006 3.584412 -0.706608  
N -1.548516 1.947641 -0.353963  
N 1.285832 1.298232 -0.598431  
C 1.573902 -0.973807 -1.272038  
C 1.115525 -2.258840 -1.515338  
H 1.802988 -3.026342 -1.856547  
C -0.243025 -2.565459 -1.334149  
C -1.116684 -1.596481 -0.876944  
H -2.162412 -1.841956 -0.733483  
H 2.624564 -0.734567 -1.406572  
O -1.104537 3.851092 -1.589633  
C -2.713679 0.244060 0.841538  
C -2.479494 -0.734724 1.829106  
C -3.983671 0.853870 0.755497  
C -3.492088 -1.080107 2.720807  
H -1.500576 -1.195789 1.915609  
C -4.995278 0.488211 1.639333  
H -4.195523 1.571872 -0.033116  
C -4.748983 -0.473083 2.626318  
H -3.300810 -1.821229 3.490975  
H -5.977335 0.943245 1.552720  
H -5.538714 -0.753038 3.317523  
H -0.787373 1.951439 -2.301308  
Cl -0.823966 -4.171980 -1.678392  
H -0.356860 4.435029 -1.329186

H 2.314104 1.289628 -0.413717  
H -2.143637 2.618935 0.129918  
O 4.035663 1.055168 -0.314009  
H 4.448643 0.784888 0.547295  
H 4.561439 1.800447 -0.643112  
O 5.099822 0.259111 2.061489  
H 5.132035 0.854160 2.825409  
H 5.924228 -0.275078 2.098210  
O 7.457744 -1.226511 2.263926  
H 8.321522 -1.034073 1.867732  
H 7.528496 -2.108465 2.660402

\*\*\*\*

**Cat3 4w**

C 1.029957 0.334436 -0.651105  
C -0.311787 0.086132 -1.077189  
C 1.898597 -0.692920 -0.097802  
C -0.425701 -2.371048 -1.374128  
C 1.075078 -2.391272 -1.730965  
O -1.054046 -3.419048 -1.403094  
N 1.824578 -1.932170 -0.543347  
N -0.948573 -1.160587 -1.037954  
C -1.106776 1.180856 -1.469948  
C -0.596462 2.468541 -1.505623  
H -1.223748 3.293305 -1.828599  
C 0.737917 2.705390 -1.136525  
C 1.531593 1.661526 -0.700470  
H 2.558260 1.853043 -0.411509  
H -2.139360 0.994348 -1.749512  
O 1.484928 -3.672157 -2.027508  
C 2.876904 -0.411481 0.963056  
C 2.547380 0.455764 2.024616  
C 4.137700 -1.045158 0.949653  
C 3.457449 0.668991 3.057259  
H 1.572650 0.932628 2.053601  
C 5.048008 -0.811183 1.976954  
H 4.425501 -1.676494 0.112437  
C 4.707046 0.040469 3.033829  
H 3.191980 1.324593 3.881127  
H 6.025807 -1.282465 1.948551  
H 5.417809 0.218711 3.835641  
H 1.296324 -1.695571 -2.552146  
Cl 1.388895 4.320460 -1.220385  
H 0.697293 -4.252138 -1.920085  
H -1.994766 -1.133433 -0.974101  
H 2.342703 -2.672953 -0.072757  
O -3.678403 -0.824597 -1.039053  
H -4.144388 -0.550040 -0.196891  
H -4.215181 -1.527795 -1.434849  
O -4.831834 0.006823 1.225777  
H -5.365952 0.825551 1.154499  
H -5.328941 -0.603866 1.807704  
O -6.275805 -1.736510 2.944157  
H -5.992229 -1.947967 3.846796  
H -6.924771 -2.413850 2.699217  
O -6.378910 2.378146 1.019226  
H -6.511862 2.955861 1.786543  
H -7.199235 2.424500 0.504267

\*\*\*\*

**TS Cat3 -> Cat1 0w**

C -0.563604 0.265813 0.096813  
C -2.024712 0.196031 0.094307  
C 0.308113 -0.841392 -0.052281  
C -2.160915 -2.050867 0.809517  
C -1.307845 -2.744847 -0.278145  
O -2.226276 -2.513431 1.921061  
N -0.049899 -2.146712 -0.316052  
N -2.757327 -0.930433 0.281084  
C -2.757300 1.395932 -0.135059  
C -2.137317 2.616803 -0.194401  
H -2.720863 3.524385 -0.314315  
C -0.721291 2.706774 -0.073058  
C 0.039401 1.580155 0.059370  
H 1.116319 1.672101 0.080426  
H -3.838946 1.317341 -0.173384  
C 1.788350 -0.700700 -0.011139  
C 2.570232 -1.105426 -1.109235  
C 2.416767 -0.235908 1.158785  
C 3.961955 -1.029285 -1.040715  
H 2.093742 -1.433133 -2.030856  
C 3.808673 -0.183423 1.224812  
H 1.819203 0.058871 2.016815  
C 4.581837 -0.573776 0.126478  
H 4.559431 -1.318975 -1.900049  
H 4.288843 0.161415 2.135756  
H 5.665304 -0.521447 0.180018  
Cl 0.027956 4.278040 -0.143996  
H 0.740952 -2.768202 -0.461046  
O -2.113095 -2.371692 -1.609240  
H -2.644572 -3.117989 -1.963550  
H -1.255980 -3.831280 -0.270494  
H -2.747220 -1.624072 -1.157471

\*\*\*\*

## XYZ coordinates for Table S5

**4cis 0w**

C -0.035491 0.076556 -0.441939  
 C -1.456087 -0.037299 -0.432395  
 C 0.867411 -1.101745 -0.591678  
 C -3.271661 -1.694758 0.015647  
 C -2.234644 1.130095 -0.364041  
 C -1.651233 2.389885 -0.252426  
 H -2.272485 3.278082 -0.202466  
 C -0.262180 2.495716 -0.248247  
 C 0.532549 1.358409 -0.352103  
 H 1.610552 1.467255 -0.373059  
 H -3.314499 1.060284 -0.446461  
 C 2.276060 -1.012540 -0.087544  
 C 2.555860 -0.589190 1.222245  
 C 3.336348 -1.425555 -0.911057  
 C 3.866678 -0.597062 1.702137  
 H 1.745105 -0.269124 1.871140  
 C 4.649030 -1.415127 -0.435466  
 H 3.132791 -1.733777 -1.933858  
 C 4.916403 -1.005373 0.873717  
 H 4.067985 -0.282027 2.722543  
 H 5.461553 -1.722410 -1.088445  
 H 5.937437 -1.000800 1.245776  
 O -3.796001 -2.762259 -0.263177  
 O -5.063313 -0.615653 1.227544  
 C -3.876551 -0.820231 1.129397  
 H -3.158077 -0.448048 1.890069  
 N 0.413041 -2.165197 -1.161453  
 H 1.116037 -2.907711 -1.187785  
 Cl 0.495235 4.075706 -0.137832  
 N -2.072836 -1.292982 -0.525898  
 H -1.527272 -2.008854 -1.015278

\*\*\*\*

**4cis 1w**

C 0.216509 0.320307 -0.379392  
 C -1.183668 0.574001 -0.322934  
 C 0.781159 -1.062145 -0.432021  
 C -3.302520 -0.532488 0.378207  
 C -1.644491 1.898505 -0.366819  
 C -0.760112 2.974716 -0.408290  
 H -1.136286 3.991845 -0.442470  
 C 0.609346 2.723941 -0.446395  
 C 1.090255 1.417080 -0.443553  
 H 2.158983 1.246441 -0.501377  
 H -2.710782 2.095438 -0.416245  
 C 2.185727 -1.301507 0.029627  
 C 2.635593 -0.826951 1.272822  
 C 3.052468 -2.076818 -0.758309  
 C 3.918738 -1.138931 1.725383  
 H 1.974580 -0.228595 1.894088  
 C 4.341722 -2.372524 -0.312210  
 H 2.721194 -2.430622 -1.731673  
 C 4.775691 -1.908454 0.932831  
 H 4.249188 -0.779855 2.696377  
 H 5.006768 -2.961544 -0.938000  
 H 5.777593 -2.142474 1.282773

O -4.089120 -1.470151 0.268090  
 O -4.719829 1.057965 1.512731  
 C -3.616165 0.582626 1.391172  
 H -2.778825 0.873300 2.058975  
 N 0.034059 -2.006416 -0.887680  
 H 0.498505 -2.916999 -0.866356  
 Cl 1.741251 4.062147 -0.525595  
 N -2.097897 -0.493863 -0.262977  
 H -1.763507 -1.362961 -0.698821  
 O -3.625195 -3.970268 -1.114330  
 H -4.498318 -4.381099 -1.192841  
 H -3.781861 -3.125939 -0.647367

\*\*\*\*

**4cis 2w**

C 1.080997 -0.504256 -0.204855  
 C 0.509065 0.541552 -0.957357  
 C 0.433973 -1.853842 -0.106626  
 C -1.761541 1.102329 -1.840520  
 C 1.126571 1.797601 -0.986644  
 C 2.289378 2.035803 -0.254035  
 H 2.759080 3.013651 -0.269875  
 C 2.864152 0.989260 0.465883  
 C 2.281199 -0.278148 0.478300  
 H 2.748573 -1.087794 1.027463  
 H 0.716328 2.583366 -1.614932  
 C -0.952434 -1.935603 0.444043  
 C -1.845039 -2.922183 -0.009374  
 C -1.372961 -1.050607 1.451462  
 C -3.126519 -3.020998 0.532158  
 H -1.550153 -3.593840 -0.812544  
 C -2.651181 -1.158594 2.001966  
 H -0.692663 -0.287502 1.819474  
 C -3.531558 -2.141690 1.541404  
 H -3.812751 -3.776061 0.158310  
 H -2.958816 -0.469864 2.783908  
 H -4.531215 -2.217363 1.960569  
 O -2.608859 0.973512 -2.709350  
 O -2.545310 3.151476 -0.843801  
 C -1.951209 2.105657 -0.690207  
 H -1.580705 1.799829 0.304606  
 N 1.133499 -2.873553 -0.460379  
 H 0.632483 -3.749757 -0.283952  
 Cl 4.343404 1.264425 1.360764  
 N -0.653625 0.297258 -1.739451  
 H -0.624132 -0.459002 -2.417793  
 O 3.952493 -2.607991 -1.236224  
 H 4.271895 -3.368992 -1.742003  
 H 3.004842 -2.784367 -1.048517  
 O -2.589342 3.557685 1.997578  
 H -2.749912 3.753543 1.054928  
 H -2.859069 4.347856 2.486965

\*\*\*\*

**4cis 3w**

C 0.078993 0.430300 0.121441  
 C 1.389765 -0.033330 -0.167525  
 C -1.082480 -0.495826 0.268581

C 2.558381 -1.985768 -1.221942  
 C 2.450542 0.882628 -0.195464  
 C 2.233805 2.244427 -0.005825  
 H 3.068647 2.937060 -0.018223  
 C 0.941840 2.698695 0.249532  
 C -0.121897 1.804730 0.321210  
 H -1.116284 2.174130 0.546499  
 H 3.468599 0.522679 -0.299926  
 C -2.416965 -0.058765 -0.246904  
 C -3.582860 -0.352662 0.481229  
 C -2.533333 0.611602 -1.476625  
 C -4.835767 0.015326 -0.011144  
 H -3.505486 -0.851546 1.443140  
 C -3.788917 0.959336 -1.977539  
 H -1.640035 0.848990 -2.047174  
 C -4.942511 0.666757 -1.244163  
 H -5.727414 -0.199730 0.571985  
 H -3.865207 1.465003 -2.936423  
 H -5.918752 0.951819 -1.627514  
 O 2.769043 -3.190368 -1.217550  
 O 4.381385 -1.250830 -2.623519  
 C 3.236540 -1.089580 -2.273826  
 H 2.585288 -0.327853 -2.750630  
 N -0.896907 -1.638779 0.838198  
 H -1.741052 -2.222140 0.849343  
 Cl 0.651979 4.411314 0.509926  
 N 1.621327 -1.400184 -0.406397  
 H 1.014849 -2.045804 0.095073  
 O 0.779862 -2.013967 3.180670  
 H 0.213321 -1.914852 2.379264  
 H 1.173707 -2.897352 3.120081  
 O 2.794349 -0.028280 3.041716  
 H 2.096275 -0.711582 3.147580  
 H 2.903962 0.366128 3.918965  
 O -3.214622 -3.681482 0.778771  
 H -3.787529 -3.672646 -0.003838  
 H -2.968448 -4.609694 0.913535

\*\*\*\*

**4cis 4w**

C -0.933758 0.335481 0.189891  
 C 0.218833 1.101095 -0.130150  
 C -0.908332 -1.153021 0.287092  
 C 2.407729 0.921990 -1.310781  
 C 0.154044 2.500074 -0.067976  
 C -1.040564 3.154398 0.222470  
 H -1.071335 4.237558 0.274824  
 C -2.180650 2.400583 0.493333  
 C -2.127534 1.009708 0.490504  
 H -3.016717 0.441053 0.738500  
 H 1.064794 3.079136 -0.171603  
 C -2.121859 -1.926680 -0.118114  
 C -2.545982 -3.020763 0.655249  
 C -2.823109 -1.612093 -1.294267  
 C -3.643156 -3.786272 0.258714  
 H -2.033220 -3.254449 1.585306  
 C -3.907996 -2.390932 -1.699850  
 H -2.508159 -0.767042 -1.899998  
 C -4.322749 -3.476825 -0.923219



H -3.971093 -4.618715 0.875462  
H -4.431562 -2.146924 -2.620292  
H -5.175187 -4.074844 -1.234184  
O 3.519847 0.401283 -1.373483  
O 2.848701 2.808459 -2.743688  
C 2.034277 2.028640 -2.312283  
H 0.984972 2.024770 -2.669959  
N 0.161273 -1.719546 0.734695  
H 0.077253 -2.739325 0.728171  
Cl -3.692805 3.206714 0.874571  
N 1.420838 0.461832 -0.488262  
H 1.622693 -0.404375 0.008237  
O 2.426711 -0.670422 2.583600  
H 1.622046 -1.053339 2.187280  
H 3.167463 -1.002101 2.022161  
O 2.513819 2.095466 2.072283  
H 2.476172 1.143200 2.330426  
H 3.324680 2.434753 2.478180  
O 5.445823 -3.881450 -0.038567  
H 6.168685 -3.785883 -0.678034  
H 5.853120 -4.245615 0.762846  
O 4.383191 -1.321623 0.735823  
H 4.213087 -0.751737 -0.043058  
H 4.675315 -2.192256 0.401567

\*\*\*\*

#### 4trans 0w

C 0.112176 0.251193 -0.190029  
C 1.519356 0.456200 -0.047145  
C -0.515465 -1.096477 -0.297055  
C 3.720444 -0.670287 0.225453  
C 2.014297 1.767498 0.074393  
C 1.161905 2.866468 0.022261  
H 1.564934 3.870513 0.108148  
C -0.205851 2.667279 -0.150898  
C -0.722621 1.381453 -0.248859  
H -1.789420 1.250421 -0.382669  
H 3.077641 1.914775 0.204110  
C -1.987788 -1.246295 -0.048205  
C -2.570109 -0.826303 1.159003  
C -2.788798 -1.891925 -1.003666  
C -3.923243 -1.061235 1.408791  
H -1.959971 -0.328031 1.907648  
C -4.146603 -2.109619 -0.759328  
H -2.349555 -2.206344 -1.947455  
C -4.715620 -1.698728 0.449032  
H -4.359055 -0.744223 2.352555  
H -4.758451 -2.597405 -1.513538  
H -5.771076 -1.871816 0.641673  
O 4.458155 0.273900 0.501488  
O 3.709545 -3.079168 -0.104364  
C 4.333373 -2.073567 0.150980  
H 5.420265 -2.073261 0.359233  
N 0.215695 -2.116141 -0.595517  
H -0.324146 -2.983989 -0.607103  
Cl -1.290414 4.047291 -0.241537  
N 2.384005 -0.646900 -0.032156  
H 1.933660 -1.545072 -0.268134

\*\*\*\*

#### 4trans 1w

C -0.454614 0.440021 -0.195399  
C 0.745142 1.202341 -0.050096  
C -0.476545 -1.046519 -0.302316  
C 3.210470 1.068536 0.243519  
C 0.662040 2.601240 0.070461  
C -0.565095 3.255899 0.015592  
H -0.607591 4.336934 0.100599  
C -1.731906 2.515290 -0.159079  
C -1.678154 1.130292 -0.256614  
H -2.597974 0.574784 -0.391991  
H 1.571688 3.170723 0.202538  
C -1.757708 -1.784913 -0.048107  
C -2.455328 -1.637633 1.161981  
C -2.228640 -2.703322 -1.000108  
C -3.592383 -2.405671 1.418506  
H -2.099140 -0.932348 1.908093  
C -3.377112 -3.457353 -0.748963  
H -1.703986 -2.811429 -1.946449  
C -4.058559 -3.313529 0.462567  
H -4.115395 -2.292988 2.364444  
H -3.739563 -4.153867 -1.500362  
H -4.949542 -3.903475 0.660352  
O 3.497864 2.228104 0.533163  
O 4.180241 -1.127376 -0.114733  
C 4.342657 0.042407 0.171395  
H 5.334373 0.468395 0.405210  
N 0.606923 -1.678231 -0.604236  
H 0.467341 -2.690783 -0.614706  
Cl -3.284846 3.331389 -0.251665  
N 1.984644 0.546599 -0.031756  
H 1.938555 -0.455398 -0.276308  
O 6.806414 -2.370486 0.042114  
H 5.865386 -2.142016 -0.075356  
H 6.955504 -3.165184 -0.490204

\*\*\*\*

#### 4trans 2w

C -0.603748 -0.279208 0.302299  
C 0.739257 -0.756231 0.215643  
C -0.960861 1.167571 0.356294  
C 3.093587 -0.024926 -0.147062  
C 0.978933 -2.138404 0.163626  
C -0.070280 -3.052416 0.214985  
H 0.142417 -4.115585 0.176683  
C -1.378663 -2.588574 0.323872  
C -1.642548 -1.223962 0.361535  
H -2.667930 -0.885774 0.448570  
H 1.988489 -2.514439 0.090813  
C -2.351149 1.595872 -0.007673  
C -2.922491 1.238851 -1.240139  
C -3.069143 2.434644 0.859981  
C -4.179519 1.725827 -1.602369  
H -2.376188 0.591808 -1.921095  
C -4.334948 2.905001 0.503826  
H -2.642693 2.700465 1.824352  
C -4.890584 2.555676 -0.730031

H -4.604456 1.454350 -2.565031  
H -4.886885 3.540457 1.191333  
H -5.873694 2.925056 -1.009395  
O 3.648748 -1.066230 -0.506090  
O 3.522262 2.323024 0.286597  
C 3.948260 1.241414 -0.066398  
H 5.000405 1.081817 -0.360632  
N -0.065696 2.026415 0.709667  
H -0.421422 2.984207 0.678431  
Cl -2.711496 -3.728845 0.410271  
N 1.798269 0.170293 0.193248  
H 1.519878 1.131417 0.451547  
O 5.957189 3.846107 -0.018638  
H 5.035609 3.601724 0.186024  
H 6.097459 4.720797 0.371326  
O 3.746926 -3.939032 -0.809346  
H 4.619960 -4.344074 -0.705225  
H 3.898847 -2.976598 -0.823239

\*\*\*\*

#### 4trans 3w

C 0.579965 0.420444 0.159520  
C -0.774629 0.867647 0.110102  
C 0.973717 -1.013810 0.086731  
C -3.106963 0.106946 -0.340351  
C -1.049924 2.242386 0.173249  
C -0.023653 3.174286 0.305547  
H -0.263609 4.231011 0.358429  
C 1.296911 2.737317 0.376684  
C 1.595789 1.381773 0.298107  
H 2.628795 1.061039 0.358033  
H -2.068312 2.598894 0.129750  
C 2.349796 -1.378430 -0.373333  
C 2.872328 -0.886709 -1.580951  
C 3.107759 -2.284433 0.388605  
C 4.123861 -1.311601 -2.029291  
H 2.292954 -0.185794 -2.175901  
C 4.368320 -2.689852 -0.054524  
H 2.719279 -2.646184 1.338135  
C 4.875664 -2.209833 -1.265363  
H 4.512901 -0.938731 -2.973024  
H 4.954576 -3.377305 0.549314  
H 5.854935 -2.530408 -1.611023  
O -3.685682 1.158407 -0.621301  
O -3.468319 -2.275986 -0.082147  
C -3.923554 -1.186633 -0.370155  
H -4.974169 -1.041787 -0.675970  
N 0.120477 -1.923048 0.430105  
H 0.498234 -2.863281 0.291426  
Cl 2.598599 3.900112 0.561663  
N -1.809841 -0.080301 0.001616  
H -1.514840 -1.051036 0.182764  
O -5.953079 -3.674634 -0.480806  
H -5.008789 -3.542451 -0.278496  
H -6.094848 -4.631753 -0.504380  
O -3.871872 4.041512 -0.552524  
H -4.749939 4.423715 -0.410966  
H -4.013777 3.088163 -0.694619  
O 0.622220 -2.705507 3.209021

H 0.026611 -2.748653 3.971523  
H 0.110872 -2.291201 2.489285

\*\*\*\*

**4trans 4w**

C 0.617709 0.153568 0.692210  
C -0.554078 0.943702 0.584852  
C 0.606735 -1.331604 0.553112  
C -2.866232 0.823384 -0.300967  
C -0.470713 2.335773 0.719959  
C 0.750280 2.954358 0.973570  
H 0.803366 4.032195 1.085366  
C 1.900152 2.175472 1.087664  
C 1.839681 0.794310 0.940047  
H 2.746132 0.205443 1.021141  
H -1.366876 2.937089 0.633073  
C 1.754710 -1.993620 -0.132005  
C 2.276813 -1.461560 -1.324774  
C 2.279079 -3.193450 0.380406  
C 3.293508 -2.141667 -1.999055  
H 1.879404 -0.536427 -1.738255  
C 3.310755 -3.853502 -0.287256  
H 1.901337 -3.591882 1.319432  
C 3.815041 -3.331597 -1.483027  
H 3.677764 -1.735656 -2.930965  
H 3.723778 -4.769158 0.127591  
H 4.615043 -3.848579 -2.006740  
O -2.965924 1.924751 -0.854960  
O -4.067894 -1.216372 0.190057  
C -4.068664 -0.120142 -0.335663  
H -4.940531 0.276723 -0.882717  
N -0.402889 -1.989487 1.020262  
H -0.317602 -2.990644 0.827633  
Cl 3.445837 2.944188 1.405346  
N -1.799196 0.319363 0.352267  
H -1.864039 -0.654557 0.658759  
O -6.726182 -1.752774 -0.762009  
H -5.905746 -1.946403 -0.273753  
H -7.353485 -2.453072 -0.532306  
O -1.076524 2.927559 -2.730152  
H -1.566153 3.011513 -3.561675  
H -1.735585 2.656573 -2.056253  
O -1.821185 -1.546846 3.611541  
H -2.719091 -1.881733 3.470617  
H -1.356455 -1.691870 2.762374  
O 1.313649 1.423097 -2.755382  
H 0.464202 1.918090 -2.766970  
H 1.993724 2.106138 -2.662137

\*\*\*\*

**TS4ax 2w**

C 0.717941 -0.433894 -0.283062  
C 0.860484 -1.738912 -0.821957  
C -0.508015 0.385477 -0.431096  
C -1.476414 -2.601185 -1.256773  
C -1.992229 -2.011804 0.053410  
H 0.184523 -3.016262 -2.298246  
H -3.083997 -1.875100 0.024845

O -2.194979 -3.265969 -1.987987  
N -1.658816 -0.192298 -0.493794  
N -0.138551 -2.405584 -1.554221  
C 2.100246 -2.390395 -0.703962  
C 3.169252 -1.815062 -0.030083  
H 4.111732 -2.344842 0.063177  
C 3.004001 -0.555578 0.550359  
C 1.804977 0.127963 0.416685  
H 1.699767 1.109322 0.863713  
H 2.210355 -3.385108 -1.128054  
O -1.396832 -2.268083 1.126671  
H -2.225520 -1.449176 2.394530  
O -2.787208 -0.848184 2.959393  
H -3.210603 -1.411001 3.623155  
H -3.641572 0.253154 1.838724  
O -3.938868 0.830082 1.091252  
H -2.482458 0.411131 -0.557726  
H -4.886085 0.979846 1.223145  
C -0.393560 1.871762 -0.518549  
C -1.331076 2.689835 0.137072  
C 0.610019 2.467108 -1.303731  
C -1.251121 4.077922 0.015461  
H -2.115552 2.243555 0.743121  
C 0.671152 3.854400 -1.436480  
H 1.332056 1.844020 -1.823359  
C -0.254897 4.663430 -0.771278  
H -1.970237 4.702157 0.539073  
H 1.442878 4.302251 -2.056822  
H -0.199761 5.744823 -0.865897  
Cl 4.327916 0.173367 1.443646

\*\*\*\*

**TS4ax 3w**

C -0.997279 0.321808 -0.335705  
C -1.473392 1.582835 -0.780189  
C 0.252966 -0.297050 -0.828075  
C 0.512177 2.774920 -1.792701  
C 1.426070 2.292828 -0.668441  
H -1.408235 2.924838 -2.351018  
H 2.484544 2.342892 -0.969903  
O 0.913463 3.519406 -2.673601  
N 1.252889 0.453077 -1.153191  
N -0.814501 2.384450 -1.729455  
C -2.723384 2.034599 -0.323728  
C -3.477621 1.305555 0.585901  
H -4.432289 1.683186 0.937492  
C -2.978040 0.090930 1.062265  
C -1.765887 -0.399068 0.600463  
H -1.399826 -1.350389 0.968372  
H -3.091934 2.995493 -0.673207  
O 1.081737 2.486013 0.523548  
H 2.332978 2.197322 1.602625  
O 3.145318 1.941269 2.131149  
H 3.551852 2.765906 2.435533  
H 3.887609 0.386113 0.927105  
O 3.877822 -0.575711 0.767451  
H 2.079626 -0.033783 -1.502177  
H 3.739251 -0.917910 1.673803  
C 0.346293 -1.777472 -0.967072

C 1.545577 -2.432059 -0.630802  
C -0.725968 -2.520025 -1.493982  
C 1.659090 -3.810843 -0.816032  
H 2.371817 -1.866155 -0.202536  
C -0.596376 -3.894514 -1.692334  
H -1.650898 -2.020035 -1.766433  
C 0.594259 -4.543145 -1.349216  
H 2.582627 -4.312032 -0.539216  
H -1.424220 -4.457999 -2.114220  
H 0.690188 -5.615803 -1.496127  
Cl -3.896668 -0.827265 2.242403  
O 3.205950 -0.454190 3.554174  
H 3.072980 0.471487 3.249016  
H 2.403327 -0.702401 4.034682

\*\*\*\*

**TS4ax 4w**

C 1.243611 -0.556781 -0.266752  
C 1.311325 -1.895473 -0.737488  
C 0.125475 0.361324 -0.558720  
C -1.047990 -2.512708 -1.398724  
C -1.623545 -1.743577 -0.209238  
H 0.661541 -3.220911 -2.175241  
H -2.693749 -1.544581 -0.380887  
O -1.748604 -3.156175 -2.165444  
N -1.070220 -0.093589 -0.740048  
N 0.332506 -2.504302 -1.535458  
C 2.472334 -2.645525 -0.477454  
C 3.527093 -2.131202 0.262909  
H 4.404226 -2.737253 0.465434  
C 3.434395 -0.830244 0.765035  
C 2.319371 -0.053611 0.495377  
H 2.267687 0.956612 0.883586  
H 2.527443 -3.666999 -0.844719  
O -1.202649 -2.020908 0.949627  
H -2.362111 -1.326182 2.091032  
O -3.120408 -0.846756 2.521446  
H -3.913179 -1.106277 2.006041  
H -3.018565 0.766512 2.255640  
O -3.052604 1.732389 1.952775  
H -1.818333 0.574715 -0.955838  
H -3.567727 2.202405 2.625338  
C 0.386985 1.826643 -0.655982  
C -0.426501 2.733468 0.044477  
C 1.419250 2.311084 -1.477996  
C -0.202112 4.106315 -0.080434  
H -1.206333 2.370123 0.709421  
C 1.621581 3.684372 -1.614695  
H 2.051276 1.612939 -2.019906  
C 0.813754 4.584788 -0.912574  
H -0.820471 4.801778 0.480929  
H 2.412222 4.050533 -2.264061  
H 0.980571 5.654410 -1.009653  
Cl 4.743302 -0.173247 1.732271  
O -3.825288 1.174560 -0.567188  
H -4.292170 1.870156 -1.053849  
H -3.644680 1.532421 0.346067  
O -5.228132 -1.010138 0.587194  
H -5.407993 -1.771603 0.016264

H -4.860460 -0.305388 0.010601

\*\*\*\*

**TS4eq 0w**

C -0.555826 0.326728 -0.004078  
 C -1.868238 0.077740 0.487350  
 C 0.453565 -0.741501 -0.123173  
 C -2.202080 -2.446881 0.326730  
 C -1.243489 -2.487496 -0.881858  
 O -2.835274 -3.382527 0.761912  
 N 0.073317 -1.945458 -0.396992  
 N -2.330525 -1.173541 0.917644  
 C -2.743839 1.172905 0.634448  
 C -2.372959 2.462098 0.281895  
 H -3.071853 3.284555 0.395495  
 C -1.095299 2.688529 -0.241755  
 C -0.198440 1.640841 -0.372972  
 H 0.792335 1.829073 -0.770581  
 H -3.743970 0.994689 1.021188  
 O -0.775374 -3.678161 -1.301907  
 C 1.899348 -0.480845 0.081718  
 C 2.340839 0.399245 1.085329  
 C 2.847941 -1.157847 -0.704722  
 C 3.705696 0.589752 1.301986  
 H 1.618196 0.915853 1.710030  
 C 4.210800 -0.953231 -0.493776  
 C 4.642621 -0.081845 0.511186  
 H 4.036591 1.261212 2.089460  
 H 4.935158 -1.472996 -1.114654  
 H 5.705299 0.073672 0.676824  
 H -3.102685 -1.148384 1.577684  
 Cl -0.626181 4.307518 -0.726270  
 H 0.389500 -3.051551 -0.743459  
 H -1.665075 -1.814004 -1.660664  
 H 2.513374 -1.830579 -1.489190

\*\*\*\*

**TS4eq 1w**

C -0.698102 -0.460176 0.010536  
 C -0.763273 -1.752277 0.597451  
 C 0.570417 0.285961 -0.089491  
 C 1.630796 -2.563370 0.541820  
 C 1.825196 -1.773559 -0.787560  
 O 2.461532 -3.270464 1.066716  
 N 1.675983 -0.327864 -0.367748  
 N 0.355145 -2.418227 1.111021  
 C -2.024156 -2.363080 0.746427  
 C -3.185616 -1.750025 0.300532  
 H -4.145282 -2.243819 0.414103  
 C -3.107245 -0.496594 -0.318771  
 C -1.886156 0.144594 -0.451437  
 H -1.838517 1.120734 -0.920797  
 H -2.080644 -3.346316 1.206226  
 O 2.996338 -1.964176 -1.402923  
 C 0.611513 1.752170 0.136351  
 C -0.239122 2.362378 1.076580  
 C 1.543236 2.542895 -0.563151  
 C -0.155795 3.733922 1.315305

H -0.948940 1.761303 1.636595  
 C 1.612795 3.914933 -0.328542  
 C 0.766151 4.513158 0.610282  
 H -0.808491 4.192456 2.053005  
 H 2.329746 4.516504 -0.880034  
 H 0.825474 5.582878 0.792691  
 H 0.179789 -3.094159 1.848670  
 H 0.955316 -2.007882 -1.431906  
 Cl -4.565737 0.268271 -0.919961  
 H 3.743598 -1.060004 -1.096547  
 H 2.717756 0.119558 -0.354221  
 O 4.105977 0.050697 -0.705768  
 H 4.747257 -0.037815 0.015777  
 H 2.207962 2.084540 -1.289338

\*\*\*\*

**TS4eq 2w**

C -0.874571 -0.568832 -0.018561  
 C -0.705609 -1.846701 0.579142  
 C 0.240535 0.389321 -0.141140  
 C 1.782860 -2.228616 0.449539  
 C 1.797104 -1.412158 -0.872105  
 H 0.494431 -2.996903 1.806095  
 O 2.745685 -2.781324 0.939626  
 N 1.442740 -0.003217 -0.428988  
 N 0.525069 -2.312697 1.055966  
 C -1.840399 -2.657789 0.775016  
 C -3.101661 -2.252083 0.364376  
 H -3.961133 -2.897842 0.512910  
 C -3.254128 -1.009226 -0.262633  
 C -2.162567 -0.174494 -0.438658  
 H -2.294694 0.794221 -0.907161  
 H -1.716875 -3.631025 1.242899  
 H 3.906361 -1.161242 -0.954614  
 O 4.850322 -0.665709 -0.324585  
 H 5.038551 -1.246989 0.428571  
 H 4.281644 0.378826 0.046632  
 O 3.532058 1.270440 0.264700  
 H 2.344293 0.675050 -0.234120  
 H 3.846640 2.053430 -0.211405  
 C 0.002362 1.837518 0.075289  
 C 0.638679 2.779646 -0.752125  
 C -0.832868 2.286907 1.113424  
 C 0.442121 4.144062 -0.543763  
 H 1.265912 2.436466 -1.569730  
 C -1.011925 3.652743 1.329293  
 H -1.321425 1.568112 1.764838  
 C -0.378293 4.583115 0.499682  
 H 0.927573 4.864122 -1.196690  
 H -1.645227 3.990545 2.144908  
 H -0.526145 5.647058 0.664314  
 Cl -4.838985 -0.504422 -0.815727  
 H 0.938352 -1.754118 -1.477066  
 O 2.929434 -1.457608 -1.570058

\*\*\*\*

**TS4eq 3w**

C -1.274572 -0.480512 -0.017682

C -1.352208 -1.773264 0.565793  
 C -0.016195 0.289221 -0.036291  
 C 1.041990 -2.559654 0.578369  
 C 1.271379 -1.707265 -0.694647  
 H -0.438138 -3.125518 1.831188  
 O 1.858976 -3.297577 1.084178  
 N 1.130542 -0.282569 -0.247817  
 N -0.245068 -2.433156 1.113498  
 C -2.611081 -2.396359 0.667634  
 C -3.759945 -1.792707 0.177962  
 H -4.718880 -2.294872 0.254928  
 C -3.669623 -0.537329 -0.436178  
 C -2.450462 0.115412 -0.520891  
 H -2.393824 1.095779 -0.980341  
 H -2.676501 -3.380256 1.124817  
 H 3.306452 -1.794054 -0.759227  
 O 4.462839 -1.333407 -0.039317  
 H 4.825634 -2.006740 0.553560  
 H 3.843143 -0.232569 0.563677  
 O 3.267543 0.681910 0.682969  
 H 2.125380 0.256450 0.078117  
 H 3.784720 1.285858 0.111805  
 C -0.035549 1.751850 0.204419  
 C 0.826105 2.588306 -0.528044  
 C -0.882814 2.315897 1.175342  
 C 0.839274 3.961842 -0.290954  
 H 1.467218 2.161521 -1.293696  
 C -0.853833 3.688049 1.419734  
 H -1.543450 1.677617 1.754688  
 C 0.004112 4.513014 0.685357  
 H 1.501627 4.600468 -0.868451  
 H -1.498726 4.113011 2.183883  
 H 0.019918 5.583352 0.872822  
 Cl -5.111275 0.215422 -1.089018  
 H 0.429122 -1.904838 -1.375866  
 O 2.426608 -1.938872 -1.349336  
 O 5.320734 0.927566 -1.267440  
 H 6.261886 1.149476 -1.232228  
 H 5.244706 -0.012750 -0.954096

\*\*\*\*

**TS4eq 4w**

C 1.358643 -0.187995 -0.245947  
 C 2.143523 -1.329259 -0.547435  
 C -0.043623 -0.008719 -0.658478  
 C 0.440511 -3.049767 -1.227749  
 C -0.620012 -2.414567 -0.326633  
 H 2.369634 -2.981357 -1.762848  
 H -1.555952 -2.933503 -0.543094  
 O 0.224210 -4.066200 -1.863001  
 N -0.880263 -1.010583 -0.744603  
 N 1.670733 -2.420801 -1.284243  
 C 3.493837 -1.352044 -0.160175  
 C 4.062869 -0.305886 0.551633  
 H 5.103629 -0.350497 0.855423  
 C 3.273521 0.796417 0.894617  
 C 1.948919 0.861375 0.493457  
 H 1.349521 1.721733 0.764846  
 H 4.096967 -2.222440 -0.404863

O -0.256295 -2.517283 1.005045  
H -1.120911 -2.403052 1.513960  
O -2.731832 -2.029022 1.797013  
H -3.289577 -2.732319 2.161682  
H -3.194256 -1.648504 0.769487  
O -3.464642 -1.104567 -0.330100  
H -1.933643 -0.860565 -0.873763  
H -4.088029 -1.637981 -0.845577  
C -0.531257 1.346899 -0.990262  
C 0.276172 2.209776 -1.761495  
C -1.809430 1.771456 -0.587705  
C -0.200960 3.463954 -2.133940  
H 1.260135 1.887664 -2.089058  
C -2.270049 3.037730 -0.944645  
H -2.449679 1.144732 0.020226  
C -1.472034 3.882241 -1.720770  
H 0.418673 4.115600 -2.743865  
H -3.255332 3.341724 -0.604292  
H -1.835778 4.866661 -2.003881  
Cl 3.967362 2.105661 1.828075  
H -2.832425 -0.524738 2.718335  
H -4.448725 0.400200 0.385302  
O -2.912365 0.409462 3.044229  
H -3.164024 0.353630 3.977384  
O -4.671535 1.215964 0.882414  
H -4.212793 1.089955 1.737613

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#### TS4rot 0w

C -0.094812 0.263884 0.576227  
C -1.515273 0.222453 0.592677  
C 0.748206 -0.939169 0.852458  
C -3.204636 -1.609045 0.138322  
C -3.709739 -0.958694 -1.168987  
H -1.708900 -1.613324 1.495363  
O -3.670314 -2.681233 0.489569  
N 0.283539 -1.839001 1.647722  
N -2.197451 -0.989408 0.848015  
C -2.233008 1.414715 0.419513  
C -1.590119 2.626680 0.181196  
H -2.164476 3.538438 0.053744  
C -0.196951 2.657139 0.144290  
C 0.541005 1.495627 0.346620  
H 1.623931 1.544898 0.336513  
H -3.314285 1.400196 0.512793  
H 0.931147 -2.625024 1.747053  
C 2.095622 -1.043474 0.208365  
C 2.264441 -0.789549 -1.162993  
C 3.203030 -1.461854 0.964734  
C 3.509302 -0.972053 -1.767387  
H 1.416245 -0.466570 -1.760327  
C 4.451688 -1.625508 0.362618  
H 3.090163 -1.635765 2.032269  
C 4.606296 -1.386039 -1.005935  
H 3.622456 -0.788774 -2.832522  
H 5.303306 -1.934872 0.962677  
H 5.577338 -1.517413 -1.475838  
Cl 0.636128 4.176354 -0.137403  
H -3.833871 0.138455 -1.207399

O -3.980956 -1.645025 -2.125687

\*\*\*\*

#### TS4rot 1w

C -0.074055 0.339968 -0.416605  
C 1.347610 0.428731 -0.465121  
C -0.822789 -0.940889 -0.575495  
C 3.330628 -1.046814 -0.088792  
C 3.944583 -0.101946 0.953914  
H 1.634398 -1.494595 -1.122749  
O 3.896855 -2.112915 -0.310700  
N -0.238502 -1.967881 -1.098868  
N 2.122559 -0.730476 -0.644936  
C 1.964452 1.685488 -0.375860  
C 1.219526 2.848306 -0.194008  
H 1.715584 3.811152 -0.128402  
C -0.169799 2.761558 -0.139642  
C -0.806268 1.530696 -0.261014  
H -1.888654 1.493994 -0.242960  
H 3.039571 1.765788 -0.493529  
H -0.878359 -2.764838 -1.152325  
C -2.256094 -1.007604 -0.141303  
C -2.630491 -0.693184 1.175385  
C -3.232188 -1.470424 -1.038508  
C -3.954003 -0.854100 1.588296  
H -1.882534 -0.341375 1.880876  
C -4.559325 -1.612029 -0.628000  
H -2.954065 -1.700602 -2.064318  
C -4.921718 -1.308553 0.687127  
H -4.228904 -0.624194 2.614140  
H -5.308300 -1.957379 -1.335514  
H -5.953241 -1.424247 1.008654  
Cl -1.129970 4.216478 0.057935  
H 3.353448 0.018703 1.886307  
O 5.034550 0.403989 0.820882  
O 1.736671 -4.004222 0.666498  
H 2.620612 -3.742541 0.353529  
H 1.126532 -3.481523 0.122328

\*\*\*\*

#### TS4rot 2w

C 0.334846 0.396904 0.374381  
C -1.073978 0.558109 0.480509  
C 1.009365 -0.924384 0.529440  
C -3.123568 -0.840827 0.158197  
C -3.721586 0.103820 -0.898873  
H -1.461672 -1.336469 1.202787  
O -3.741897 -1.867117 0.439589  
N 0.485193 -1.795656 1.326108  
N -1.901932 -0.564846 0.696982  
C -1.627006 1.843415 0.393658  
C -0.825616 2.960421 0.164339  
H -1.270842 3.948161 0.104686  
C 0.553077 2.798043 0.047150  
C 1.127394 1.535297 0.156576  
H 2.204070 1.431547 0.084810  
H -2.691594 1.982669 0.541707  
H 1.013523 -2.671690 1.326480

C 2.270185 -1.190849 -0.226348  
C 2.381413 -0.873681 -1.590630  
C 3.347982 -1.819526 0.420676  
C 3.538927 -1.201480 -2.297886  
H 1.555131 -0.387717 -2.101982  
C 4.512011 -2.127436 -0.284657  
H 3.284815 -2.038000 1.484055  
C 4.607347 -1.824839 -1.646230  
H 3.607089 -0.967361 -3.356783  
H 5.345372 -2.597477 0.230377  
H 5.512303 -2.068979 -2.196124  
Cl 1.578829 4.194943 -0.222293  
H -3.283189 0.023686 -1.911531  
O -4.663063 0.825404 -0.656566  
O -4.745404 -2.442648 -2.155499  
H -4.647323 -2.505152 -1.185515  
H -5.698177 -2.451381 -2.327986  
O 0.599664 -1.334672 4.245799  
H -0.205595 -1.525915 4.749058  
H 0.354014 -1.432100 3.304905

\*\*\*\*

#### TS4rot 3w

C 0.414637 0.376022 0.135863  
C -0.996020 0.520156 0.087220  
C 1.082922 -0.799783 0.760751  
C -2.981339 -1.003601 0.064433  
C -3.486662 -0.497811 -1.296546  
H -1.455716 -1.034711 1.377360  
O -3.610351 -1.911948 0.610475  
N 0.564910 -1.314582 1.828496  
N -1.831166 -0.504881 0.592133  
C -1.551940 1.688046 -0.446984  
C -0.743037 2.694882 -0.967741  
H -1.188664 3.600706 -1.365117  
C 0.641144 2.543954 -0.935193  
C 1.216498 1.402132 -0.388368  
H 2.296434 1.310742 -0.353906  
H -2.624668 1.836498 -0.414863  
H 1.085246 -2.139458 2.137250  
C 2.327326 -1.338747 0.136048  
C 2.436891 -1.469151 -1.258825  
C 3.391417 -1.769778 0.947363  
C 3.574673 -2.043910 -1.826526  
H 1.623161 -1.136880 -1.896834  
C 4.536764 -2.324740 0.376211  
H 3.335301 -1.639671 2.025533  
C 4.627807 -2.469295 -1.011597  
H 3.639807 -2.155635 -2.905355  
H 5.359761 -2.637266 1.013185  
H 5.518260 -2.905618 -1.456103  
Cl 1.674660 3.811523 -1.572301  
H -3.009795 -0.964871 -2.179232  
O -4.408152 0.280783 -1.396435  
O -4.492373 -3.407827 -1.645188  
H -4.410251 -3.082668 -0.727189  
H -5.442545 -3.474926 -1.818926  
O -0.854200 2.759572 2.799476  
H -0.645013 1.958128 3.326742

H -0.423258 3.493709 3.260208  
O -0.273969 0.308313 4.087997  
H -1.044212 -0.086982 4.523350  
H -0.053397 -0.282156 3.331377

\*\*\*\*

**TS4rot 4w**

C 0.617432 0.486361 0.156918  
C -0.703597 0.998059 0.111886  
C 0.982538 -0.723641 0.945707  
C -2.985802 0.019173 0.308575  
C -3.382721 0.412824 -1.122307  
H -1.490549 -0.162426 1.640971  
O -3.803458 -0.625308 0.973774  
N 0.427139 -0.902636 2.099816  
N -1.751690 0.321163 0.783069  
C -0.964338 2.178714 -0.591309  
C 0.049356 2.842435 -1.278443  
H -0.163838 3.765050 -1.807805  
C 1.343148 2.328515 -1.247179  
C 1.628465 1.165967 -0.538935  
H 2.645057 0.789483 -0.513363  
H -1.959357 2.607940 -0.569582  
H 0.721581 -1.785604 2.524351  
C 1.979755 -1.678174 0.378174  
C 1.937286 -2.042452 -0.978351  
C 2.951839 -2.257889 1.211760  
C 2.834272 -2.985118 -1.482590  
H 1.188633 -1.602536 -1.630739  
C 3.859981 -3.185323 0.700311  
H 3.017955 -1.956811 2.254644  
C 3.799278 -3.554973 -0.646784  
H 2.782043 -3.271003 -2.529655  
H 4.618753 -3.612442 1.350424  
H 4.504997 -4.279364 -1.044600  
Cl 2.635249 3.160962 -2.095089  
H -3.031946 -0.284040 -1.905991  
O -4.121206 1.347218 -1.349625  
O -4.797910 -2.985554 -0.167597  
H -4.622325 -2.169835 0.350233  
H -5.706081 -2.904753 -0.494532  
O 0.443749 3.495589 2.383075  
H 0.410094 2.763127 3.036113  
H 1.126311 4.101260 2.705882  
O 0.257288 1.224387 4.059922  
H -0.577776 1.179053 4.549367  
H 0.235516 0.483681 3.410464  
O -2.637513 -2.590355 -1.885404  
H -2.221154 -3.399956 -2.214209  
H -3.414244 -2.881543 -1.353416

\*\*\*\*

**TS4zweit 0w**

C -0.555826 0.326728 -0.004078  
C -1.868238 0.077740 0.487350  
C 0.453565 -0.741501 -0.123173  
C -2.202080 -2.446881 0.326730  
C -1.243489 -2.487496 -0.881858

O -2.835274 -3.382527 0.761912  
N 0.073317 -1.945458 -0.396992  
N -2.330525 -1.173541 0.917644  
C -2.743839 1.172905 0.634448  
C -2.372959 2.462098 0.281895  
H -3.071853 3.284555 0.395495  
C -1.095299 2.688529 -0.241755  
C -0.198440 1.640841 -0.372972  
H 0.792335 1.829073 -0.770581  
H -3.743970 0.994689 1.021188  
O -0.775374 -3.678161 -1.301907  
C 1.899348 -0.480845 0.081718  
C 2.340839 0.399245 1.085329  
C 2.847941 -1.157847 -0.704722  
C 3.705696 0.589752 1.301986  
H 1.618196 0.915853 1.710030  
C 4.210800 -0.953231 -0.493776  
C 4.642621 -0.081845 0.511186  
H 4.036591 1.261212 2.089460  
H 4.935158 -1.472996 -1.114654  
H 5.705299 0.073672 0.676824  
H -3.102685 -1.148384 1.577684  
Cl -0.626181 4.307518 -0.726270  
H 0.389500 -3.051551 -0.743459  
H -1.665075 -1.814004 -1.660664  
H 2.513374 -1.830579 -1.489190

\*\*\*\*

**TS4zweit 1w**

C -0.698102 -0.460176 0.010536  
C -0.763273 -1.752277 0.597451  
C 0.570417 0.285961 -0.089491  
C 1.630796 -2.563370 0.541820  
C 1.825196 -1.773559 -0.787560  
O 2.461532 -3.270464 1.066716  
N 1.675983 -0.327864 -0.367748  
N 0.355145 -2.418227 1.111021  
C -2.024156 -2.363080 0.746427  
C -3.185616 -1.750025 0.300532  
H -4.145282 -2.243819 0.414103  
C -3.107245 -0.496594 -0.318771  
C -1.886156 0.144594 -0.451437  
H -1.838517 1.120734 -0.920797  
H -2.080644 -3.346316 1.206226  
O 2.996338 -1.964176 -1.402923  
C 0.611513 1.752170 0.136351  
C -0.239122 2.362378 1.076580  
C 1.543236 2.542895 -0.563151  
C -0.155795 3.733922 1.315305  
H -0.948940 1.761303 1.636595  
C 1.612795 3.914933 -0.328542  
C 0.766151 4.513158 0.610282  
H -0.808491 4.192456 2.053005  
H 2.329746 4.516504 -0.880034  
H 0.825474 5.582878 0.792691  
H 0.179789 -3.094159 1.848670  
H 0.955316 -2.007882 -1.431906  
Cl -4.565737 0.268271 -0.919961  
H 3.743598 -1.060004 -1.096547

H 2.717756 0.119558 -0.354221  
O 4.105977 0.050697 -0.705768  
H 4.747257 -0.037815 0.015777  
H 2.207962 2.084540 -1.289338

\*\*\*\*

**TS4zweit 2w**

C -0.874571 -0.568832 -0.018561  
C -0.705609 -1.846701 0.579142  
C 0.240535 0.389321 -0.141140  
C 1.782860 -2.228616 0.449539  
C 1.797104 -1.412158 -0.872105  
H 0.494431 -2.996903 1.806095  
O 2.745685 -2.781324 0.939626  
N 1.442740 -0.003217 -0.428988  
N 0.525069 -2.312697 1.055966  
C -1.840399 -2.657789 0.775016  
C -3.101661 -2.252083 0.364376  
H -3.961133 -2.897842 0.512910  
C -3.254128 -1.009226 -0.262633  
C -2.162567 -0.174494 -0.438658  
H -2.294694 0.794221 -0.907161  
H -1.716875 -3.631025 1.242899  
H 3.906361 -1.161242 -0.954614  
O 4.850322 -0.665709 -0.324585  
H 5.038551 -1.246989 0.428571  
H 4.281644 0.378826 0.046632  
O 3.532058 1.270440 0.264700  
H 2.344293 0.675050 -0.234120  
H 3.846640 2.053430 -0.211405  
C 0.002362 1.837518 0.075289  
C 0.638679 2.779646 -0.752125  
C -0.832868 2.286907 1.113424  
C 0.442121 4.144062 -0.543763  
H 1.265912 2.436466 -1.569730  
C -1.011925 3.652743 1.329293  
H -1.321425 1.568112 1.764838  
C -0.378293 4.583115 0.499682  
H 0.927573 4.864122 -1.196690  
H -1.645227 3.990545 2.144908  
H -0.526145 5.647058 0.664314  
Cl -4.838985 -0.504422 -0.815727  
H 0.938352 -1.754118 -1.477066  
O 2.929434 -1.457608 -1.570058

\*\*\*\*

**TS4zweit 3w**

C 1.187098 -0.566696 0.002554  
C 1.118867 -1.861139 0.580121  
C 0.023115 0.334543 -0.054568  
C -1.321605 -2.461490 0.462905  
C 2.307288 -2.604933 0.719863  
C 3.524210 -2.118696 0.266934  
H 4.425833 -2.713395 0.372298  
C 3.577308 -0.861030 -0.347715  
C 2.432580 -0.090709 -0.464263  
H 2.488177 0.890665 -0.920832  
H 2.261554 -3.590099 1.176761

C 0.228579 1.787398 0.164355  
C -0.414498 2.730744 -0.656338  
C 1.074432 2.232369 1.198498  
C -0.206385 4.093861 -0.446432  
H -1.075448 2.398957 -1.448514  
C 1.259194 3.596206 1.417076  
H 1.568946 1.510659 1.842322  
C 0.623941 4.528919 0.590109  
H -0.701827 4.814903 -1.090222  
H 1.899543 3.930371 2.228623  
H 0.776620 5.592340 0.754343  
O -2.170779 -3.227205 0.855012  
C -1.473001 -1.524727 -0.764001  
N -1.173453 -0.119454 -0.291397  
Cl 5.104433 -0.256030 -0.956716  
N -0.063983 -2.412113 1.082972  
H 0.047253 -3.162978 1.758492  
H -0.654780 -1.774850 -1.460694  
O -2.653028 -1.600559 -1.395100  
H -2.032502 0.559992 -0.203383  
H -3.513811 -1.584184 -0.727473  
O -5.433335 0.826934 -0.350565  
H -5.768962 0.928037 -1.253553  
O -3.126886 1.647718 -0.075580  
H -4.168702 1.324117 -0.243777  
H -3.140804 2.098438 0.782602  
O -4.595915 -1.388099 0.104637  
H -5.120980 -0.375856 -0.134565  
H -5.210632 -2.131672 0.168901

H -0.035770 -2.863196 2.065152  
H -0.718685 -1.521940 -1.123669  
O -2.671373 -0.949774 -0.914738  
H -1.732268 1.216130 0.199462  
H -4.050092 -1.742486 -0.306541  
O -3.915549 1.213471 -1.500420  
O -2.602312 2.034911 0.352941  
H -3.348917 1.736529 -0.524749  
H -3.043134 1.861250 1.200473  
O -4.948183 -2.038051 0.020434  
H -4.858035 0.986289 -1.274588  
H -4.763394 -2.315110 0.930721  
O -6.304299 0.166881 -0.735991  
H -5.947036 -0.690971 -0.371506  
H -6.989120 0.477171 -0.127439  
H -3.411604 0.319452 -1.456309

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#### TS4zwit 4w

C 1.403540 -0.653933 0.037211  
C 1.137534 -1.900878 0.657671  
C 0.433654 0.466634 0.074355  
C -1.363071 -1.870992 0.904599  
C 2.146439 -2.882082 0.680679  
C 3.377935 -2.667116 0.078326  
H 4.140130 -3.439412 0.094532  
C 3.620452 -1.450110 -0.568846  
C 2.656445 -0.453802 -0.577742  
H 2.864867 0.492817 -1.063534  
H 1.945383 -3.834182 1.165178  
C 0.949270 1.850360 0.268078  
C 0.401078 2.916986 -0.464325  
C 1.972818 2.112037 1.196791  
C 0.868059 4.216899 -0.271201  
H -0.382075 2.723906 -1.190095  
C 2.425367 3.415639 1.399422  
H 2.402004 1.296805 1.772450  
C 1.876892 4.470094 0.662627  
H 0.441963 5.031506 -0.850189  
H 3.206814 3.607469 2.129781  
H 2.236715 5.484392 0.814189  
O -2.320830 -2.249130 1.555719  
C -1.446452 -1.058095 -0.421626  
N -0.842365 0.284093 -0.045479  
Cl 5.161891 -1.180691 -1.361410  
N -0.067534 -2.177091 1.317047

XYZ coordinates for Table S6

**TMZ 1ax 0w**

C -0.308743 0.314776 0.091748  
C 0.573304 -0.863702 0.353284  
C -1.610210 0.173307 -0.455185  
C -2.089508 -2.217285 0.004620  
C 0.163793 1.602506 0.408435  
H 1.154729 1.712850 0.834985  
C -0.619490 2.726563 0.182974  
C -1.891201 2.599589 -0.380191  
C -2.373327 1.333425 -0.691142  
H -3.371259 1.240698 -1.105202  
H -2.502846 3.478149 -0.558273  
N -2.153920 -1.084031 -0.803883  
C 2.018261 -0.763265 -0.009105  
C 2.455507 0.016989 -1.093136  
C 2.964907 -1.507934 0.716114  
C 3.806253 0.047627 -1.446509  
C 4.314374 -1.465354 0.370515  
H 2.623561 -2.115485 1.547847  
C 4.739859 -0.688587 -0.712967  
H 4.127050 0.646104 -2.295182  
H 5.036265 -2.038129 0.946890  
H 5.792374 -0.657591 -0.982787  
O -2.688007 -3.240486 -0.287240  
Cl -0.005872 4.316108 0.601988  
C -1.216179 -2.138377 1.275660  
N 0.171755 -1.967670 0.878589  
H 1.738594 0.587294 -1.676726  
O -1.713408 -1.232813 2.252695  
H -1.585930 -0.315583 1.962562  
H -1.310137 -3.115677 1.746418  
C -3.047205 -1.174248 -1.967698  
H -2.989793 -2.189332 -2.360840  
H -4.091308 -0.973161 -1.698096  
H -2.717358 -0.461854 -2.726473

\*\*\*\*

**TMZ 1eq 0w**

C -0.246943 0.475972 -0.125124  
C -1.550613 0.577238 0.417555  
C 0.424337 -0.844317 -0.321656  
C -2.399921 -1.703941 0.075430  
C -1.566215 -1.746557 -1.218559  
O -3.091405 -2.659994 0.405762  
N -0.176810 -1.870741 -0.811950  
N -2.279464 -0.565585 0.841483  
C -2.124576 1.848417 0.592990  
C -1.447358 3.004616 0.221897  
H -1.908653 3.978221 0.351588  
C -0.172685 2.896160 -0.338576  
C 0.424552 1.652949 -0.502721  
H 1.420578 1.584486 -0.926512  
H -3.122819 1.932262 1.009712  
O -1.972877 -2.819912 -2.008895  
C 1.863109 -0.990213 0.048015  
C 2.442122 -0.234012 1.080856

C 2.653256 -1.941279 -0.621705  
C 3.779442 -0.424538 1.436866  
H 1.844281 0.493918 1.621755  
C 3.989847 -2.122894 -0.271766  
H 2.200534 -2.531127 -1.412269  
C 4.558084 -1.365362 0.758859  
H 4.210223 0.161577 2.244527  
H 4.591003 -2.855566 -0.804043  
H 5.600637 -1.508800 1.031113  
H -1.727959 -0.832072 -1.807656  
Cl 0.684128 4.345835 -0.834052  
H -2.361183 -3.486159 -1.409327  
C -3.091801 -0.493230 2.064333  
H -4.104918 -0.127837 1.857368  
H -3.170450 -1.497935 2.480813  
H -2.601101 0.169311 2.779991

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**TMZ 1eq 1w**

C -0.145168 0.562888 -0.069794  
C 0.941834 1.070682 -0.820781  
C -0.359695 -0.903464 0.119223  
C 2.457514 -0.858767 -0.852377  
C 1.935697 -1.202780 0.553755  
O 3.320833 -1.552991 -1.378836  
N 0.593284 -1.722346 0.398641  
N 1.869678 0.214941 -1.474398  
C 1.083995 2.460459 -0.971057  
C 0.192055 3.346042 -0.376703  
H 0.323382 4.417216 -0.489375  
C -0.863194 2.839966 0.385384  
C -1.036575 1.469773 0.531636  
H -1.867344 1.090597 1.116641  
H 1.916345 2.854814 -1.544373  
O 2.787630 -2.160492 1.129464  
C -1.739581 -1.458143 -0.002869  
C -2.699741 -0.869838 -0.843175  
C -2.078922 -2.627350 0.700787  
C -3.968846 -1.437471 -0.978454  
H -2.452592 0.024342 -1.408062  
C -3.348999 -3.186263 0.572485  
H -1.332692 -3.085845 1.341686  
C -4.298709 -2.593769 -0.267762  
H -4.697082 -0.975907 -1.640241  
H -3.600292 -4.085226 1.129450  
H -5.288516 -3.031837 -0.367502  
H 1.957727 -0.316714 1.203735  
Cl -1.983614 3.945876 1.160276  
H 3.276470 -2.579581 0.391229  
C 2.373830 0.574750 -2.807712  
H 3.257839 1.220214 -2.744793  
H 2.656961 -0.343086 -3.323895  
H 1.583235 1.084725 -3.361387  
O 4.145792 -0.511437 2.993982  
H 4.241665 -0.890199 3.879506  
H 3.798584 -1.232504 2.430603

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**TMZ 1eq 2w**

C 0.653142 -0.575837 -0.009445  
C -0.209525 -1.470554 -0.688447  
C 0.289744 0.854800 0.212827  
C -2.342214 -0.244855 -0.609791  
C -1.902652 0.213014 0.798259  
O -3.399939 0.101159 -1.134758  
N -0.887689 1.226810 0.580078  
N -1.433718 -1.041187 -1.268344  
C 0.182087 -2.809899 -0.853393  
C 1.390388 -3.276360 -0.349103  
H 1.672162 -4.317062 -0.471327  
C 2.229191 -2.393416 0.335376  
C 1.871728 -1.061476 0.498988  
H 2.534881 -0.385815 1.028123  
H -0.479056 -3.500883 -1.365652  
O -2.958425 0.690629 1.572364  
C 1.328577 1.909053 0.027608  
C 2.366036 1.764392 -0.908760  
C 1.248114 3.098139 0.773674  
C 3.299713 2.785997 -1.097299  
H 2.436987 0.859265 -1.505113  
C 2.187208 4.111849 0.591961  
H 0.443024 3.209624 1.493051  
C 3.215870 3.959918 -0.344853  
H 4.091204 2.663072 -1.831982  
H 2.119565 5.021069 1.183746  
H 3.947346 4.751513 -0.485691  
H -1.509200 -0.654974 1.344005  
Cl 3.748863 -2.973233 0.992822  
H -3.406863 1.450598 1.125876  
C -1.824524 -1.563714 -2.586343  
H -2.410470 -2.485634 -2.494484  
H -2.441841 -0.814451 -3.082616  
H -0.925600 -1.755149 -3.175113  
O -4.247384 -1.832337 1.944723  
H -5.089553 -1.853899 1.467387  
H -3.976786 -0.891342 1.940588  
O -4.411550 2.440831 -0.002336  
H -4.272327 1.717777 -0.649992  
H -3.973222 3.223322 -0.368422

\*\*\*\*

**TMZ An1 0w**

C -0.227627 0.446676 0.054493  
C -1.608199 0.431055 0.382503  
C 0.534678 -0.795151 -0.092793  
C -2.390036 -1.812400 -0.021200  
C -1.258637 -2.199641 -0.836647  
O -3.454529 -2.476181 -0.036112  
N -0.006444 -1.882083 -0.672411  
N -2.182857 -0.779215 0.911643  
C -2.380944 1.593979 0.289176  
C -1.814806 2.826039 -0.051909  
H -2.409209 3.733379 -0.077394  
C -0.449434 2.846498 -0.342454  
C 0.329766 1.701518 -0.310000  
H 1.375556 1.757426 -0.588885  
H -3.438476 1.552411 0.533430

O -1.535582 -3.269250 -1.683315  
C 1.989275 -0.837102 0.112407  
C 2.658784 0.044482 0.997776  
C 2.789147 -1.821272 -0.523635  
C 4.035440 -0.033689 1.210456  
H 2.083443 0.785992 1.545576  
C 4.162525 -1.894860 -0.309763  
H 2.295321 -2.525389 -1.185396  
C 4.808699 -1.000225 0.556711  
H 4.506048 0.662107 1.904076  
H 4.740365 -2.660345 -0.826709  
H 5.882020 -1.062136 0.724165  
Cl 0.305702 4.394372 -0.794407  
H -2.459121 -3.508880 -1.467108  
C -3.202963 -0.654565 1.944033  
H -4.187638 -0.345980 1.559247  
H -3.334660 -1.625543 2.428308  
H -2.858598 0.077111 2.681467

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**TMZ An1 1w**

C -0.253665 0.515558 -0.048764  
C 1.096212 0.792289 -0.376371  
C -0.733594 -0.865217 0.097017  
C 2.329206 -1.218221 0.060368  
C 1.313003 -1.844928 0.856847  
O 3.526892 -1.629590 0.109669  
N 0.017405 -1.810390 0.674266  
N 1.914520 -0.273805 -0.893052  
C 1.604801 2.093213 -0.285373  
C 0.786716 3.173939 0.054383  
H 1.173050 4.187649 0.078105  
C -0.551010 2.904328 0.348089  
C -1.067477 1.618248 0.317422  
H -2.101749 1.448781 0.593985  
H 2.647395 2.276756 -0.527814  
O 1.796465 -2.821825 1.722519  
C -2.148868 -1.211204 -0.120349  
C -2.972347 -0.498331 -1.024635  
C -2.733657 -2.327199 0.528192  
C -4.301525 -0.860958 -1.246931  
H -2.554905 0.338637 -1.577992  
C -4.060495 -2.684855 0.305818  
H -2.112233 -2.903608 1.205866  
C -4.865263 -1.955321 -0.581712  
H -4.898086 -0.287676 -1.955199  
H -4.475468 -3.543437 0.832314  
H -5.901192 -2.238676 -0.755727  
Cl -1.618322 4.254389 0.796982  
H 2.750831 -2.873062 1.517479  
C 2.872094 0.047869 -1.946117  
H 3.762896 0.586314 -1.591911  
H 3.212270 -0.882587 -2.408428  
H 2.359737 0.656207 -2.697985  
O 6.032983 -0.463907 -0.195967  
H 6.252764 -0.373807 0.742355  
H 5.137199 -0.879414 -0.189329

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**TMZ An1 2w**

C 0.617615 0.504830 -0.030198  
C -0.769356 0.703657 0.171386  
C 1.188061 -0.848165 -0.099624  
C -1.836056 -1.381775 -0.329115  
C -0.722037 -1.961150 -1.013505  
O -3.004115 -1.858165 -0.483127  
N 0.550073 -1.847515 -0.713333  
N -1.559775 -0.403625 0.643072  
C -1.346498 1.967132 -0.001939  
C -0.567757 3.087501 -0.301382  
H -1.010806 4.074096 -0.389279  
C 0.805138 2.896216 -0.468417  
C 1.393842 1.646221 -0.354268  
H 2.457313 1.535693 -0.532928  
H -2.415587 2.092310 0.142950  
O -1.061769 -2.975466 -1.903344  
C 2.597999 -1.101048 0.251790  
C 3.285295 -0.328319 1.216864  
C 3.308593 -2.180698 -0.326543  
C 4.608944 -0.601953 1.565217  
H 2.765284 0.484973 1.716047  
C 4.629591 -2.449715 0.021057  
H 2.790210 -2.800767 -1.050777  
C 5.299499 -1.662427 0.968831  
H 5.100129 0.014109 2.316907  
H 5.146106 -3.282963 -0.453431  
H 6.330994 -1.876418 1.240534  
Cl 1.823742 4.298759 -0.860284  
H -2.025872 -3.086061 -1.789328  
C -2.611777 -0.127432 1.611107  
H -3.494557 0.371024 1.181387  
H -2.944781 -1.071176 2.051339  
H -2.193912 0.508470 2.397949  
O -5.618863 -1.145615 -0.348513  
H -5.770342 -0.902039 -1.273038  
H -4.656749 -1.391651 -0.308439  
O -6.690273 0.737587 1.445010  
H -5.972189 0.904929 2.072394  
H -6.327353 0.060556 0.826604

\*\*\*\*

**TMZ An2 0w**

C -0.293154 0.423036 -0.134836  
C -1.603455 0.412498 0.413267  
C 0.474951 -0.844789 -0.336908  
C -2.269457 -1.977459 0.059011  
C -1.491132 -1.938850 -1.322904  
O -2.927824 -2.914250 0.473007  
N -0.035085 -1.920565 -0.812799  
N -2.226991 -0.774262 0.834706  
C -2.263721 1.646659 0.600559  
C -1.679101 2.855901 0.237700  
H -2.213588 3.790862 0.376280  
C -0.403165 2.844776 -0.324189  
C 0.284133 1.650923 -0.500322  
H 1.282595 1.659891 -0.925121  
H -3.267335 1.655937 1.013046

O -1.757870 -2.880646 -2.159455  
C 1.926890 -0.865921 0.043415  
C 2.450336 -0.078230 1.083453  
C 2.796496 -1.747902 -0.624848  
C 3.798716 -0.166408 1.444294  
H 1.795938 0.599672 1.624863  
C 4.142328 -1.830289 -0.271349  
H 2.380751 -2.370219 -1.411676  
C 4.653154 -1.039160 0.766181  
H 4.178866 0.447122 2.258966  
H 4.797841 -2.515001 -0.806040  
H 5.703482 -1.105423 1.042744  
Cl 0.350362 4.374017 -0.807975  
C -3.120087 -0.719727 1.990488  
H -4.141946 -0.412107 1.720667  
H -3.179140 -1.723668 2.413372  
H -2.719486 -0.022419 2.732787  
H -1.676440 -0.890338 -1.704153

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**TMZ An2 1w**

C 0.149020 0.618036 0.031932  
C -0.837775 1.417108 0.665587  
C 0.062766 -0.874221 0.042443  
C -2.735529 -0.201495 0.865533  
C -2.304133 -0.795838 -0.524798  
O -3.711525 -0.546903 1.504840  
N -1.021284 -1.527788 -0.162418  
N -1.916455 0.850975 1.368986  
C -0.687105 2.819960 0.640515  
C 0.382065 3.431084 -0.006224  
H 0.469472 4.513104 -0.026042  
C 1.329071 2.631708 -0.646063  
C 1.220937 1.247875 -0.623428  
H 1.971791 0.639056 -1.116036  
H -1.436710 3.444408 1.115368  
O -3.202930 -1.547166 -1.105197  
C 1.312342 -1.660617 0.310556  
C 2.351142 -1.173727 1.122009  
C 1.434287 -2.956873 -0.222065  
C 3.478120 -1.956068 1.393032  
H 2.273386 -0.181025 1.557062  
C 2.561132 -3.734230 0.040900  
H 0.619376 -3.335423 -0.831415  
C 3.591158 -3.238218 0.850223  
H 4.266054 -1.561461 2.031474  
H 2.637886 -4.731924 -0.386514  
H 4.469821 -3.846045 1.055796  
Cl 2.686896 3.393472 -1.487348  
C -2.409366 1.535635 2.563549  
H -3.142630 2.320439 2.325677  
H -2.909194 0.795971 3.190519  
H -1.568390 1.979564 3.104434  
H -1.987680 0.095228 -1.131196  
O -2.920409 -1.832521 -3.725325  
H -2.412776 -2.656848 -3.734022  
H -3.073348 -1.674367 -2.732909

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**TMZ An2 2w**

C 0.727943 0.504434 0.054741  
C 0.178026 1.625879 0.726061  
C -0.007922 -0.794645 -0.015335  
C -2.233214 1.003249 0.837959  
C -2.067404 0.345956 -0.575804  
O -3.283502 1.079123 1.454549  
N -1.262575 -0.886833 -0.264355  
N -1.060084 1.561672 1.396751  
C 0.925430 2.820373 0.773501  
C 2.169400 2.929289 0.161148  
H 2.721901 3.863144 0.196152  
C 2.685799 1.825356 -0.517780  
C 1.982361 0.629630 -0.567239  
H 2.401258 -0.223059 -1.091089  
H 0.511907 3.687201 1.278564  
O -3.199746 0.100061 -1.209151  
C 0.752582 -2.066646 0.215177  
C 1.896467 -2.125315 1.028758  
C 0.279202 -3.259658 -0.360387  
C 2.551838 -3.339087 1.258272  
H 2.270946 -1.219943 1.498476  
C 0.936278 -4.468433 -0.137238  
H -0.617590 -3.211391 -0.970260  
C 2.077810 -4.515253 0.672764  
H 3.431351 -3.362811 1.898374  
H 0.556761 -5.378990 -0.595848  
H 2.589265 -5.459507 0.846951  
Cl 4.257090 1.952656 -1.317734  
C -1.225474 2.313276 2.641921  
H -0.281805 2.314365 3.194400  
H -1.544900 3.350155 2.464434  
H -2.002131 1.822749 3.230222  
H -1.396326 1.037281 -1.143102  
O -2.997791 0.372103 -3.858015  
H -3.130669 -0.546101 -4.134279  
H -3.099553 0.325394 -2.854490  
O -5.339262 -0.873072 0.223392  
H -5.143627 -0.292275 0.975425  
H -4.591020 -0.621405 -0.384527

\*\*\*\*

**TMZ Cat1 0w**

C -0.176837 0.516053 -0.105585  
C -1.477348 0.793568 0.386221  
C 0.352820 -0.864577 -0.291005  
C -2.619971 -1.330476 0.074442  
C -1.716269 -1.545317 -1.160495  
O -3.447608 -2.218066 0.315951  
N -0.374086 -1.819528 -0.788045  
N -2.379988 -0.236137 0.814267  
C -1.896318 2.124651 0.518255  
C -1.068730 3.180136 0.149705  
H -1.413068 4.204541 0.246030  
C 0.204281 2.908949 -0.359863  
C 0.647577 1.595430 -0.476233  
H 1.639553 1.397950 -0.866423  
H -2.886646 2.342656 0.903501

O -2.216153 -2.746994 -1.690509  
C 1.753526 -1.171358 0.063800  
C 2.398316 -0.492327 1.116052  
C 2.445374 -2.190180 -0.620009  
C 3.701415 -0.831520 1.478378  
H 1.875667 0.282381 1.668806  
C 3.751839 -2.513255 -0.265604  
C 4.381927 -1.836910 0.786001  
H 4.184436 -0.311037 2.300090  
H 4.283183 -3.288204 -0.810400  
H 5.401042 -2.092145 1.062278  
H -1.843475 -0.771518 -1.927135  
Cl 1.243790 4.217695 -0.846256  
H -1.510179 -3.396142 -1.733016  
H -2.920436 -3.076559 -1.127506  
H 1.957676 -2.709440 -1.438596  
C -3.202047 -0.038809 2.028846  
H -4.136227 0.478875 1.790781  
H -3.440077 -1.018046 2.444655  
H -2.624607 0.541663 2.748759

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**TMZ Cat1 1w**

C -0.725113 -0.342513 -0.079969  
C -0.722948 -1.685149 0.374790  
C 0.493924 0.510361 -0.123662  
C 1.641695 -2.263990 0.276662  
C 1.766786 -1.287245 -0.915387  
O 2.659628 -2.881850 0.605532  
N 1.653879 0.068757 -0.498043  
N 0.447851 -2.322265 0.897199  
C -1.921016 -2.414030 0.377053  
C -3.107745 -1.852085 -0.081040  
H -4.023132 -2.434528 -0.084415  
C -3.108394 -0.534533 -0.547924  
C -1.935877 0.212630 -0.537715  
H -1.950729 1.236438 -0.893970  
H -1.927376 -3.439300 0.730666  
O 3.095619 -1.499058 -1.349169  
C 0.390207 1.943366 0.241326  
C -0.430604 2.358795 1.305329  
C 1.147226 2.902969 -0.455814  
C -0.474187 3.702897 1.676726  
H -1.016699 1.630366 1.858269  
C 1.084666 4.247494 -0.095602  
C 0.279115 4.649028 0.976186  
H -1.098374 4.011217 2.510345  
H 1.653302 4.985090 -0.654904  
H 0.232991 5.697033 1.258268  
H 1.105400 -1.560474 -1.746900  
Cl -4.583616 0.178598 -1.138985  
H 3.584383 -0.671568 -1.311732  
H 3.515660 -2.137211 -0.751485  
H 1.751657 2.590381 -1.302634  
C 0.334649 -3.226491 2.062230  
H 0.094598 -4.246816 1.747385  
H 1.293213 -3.237856 2.581081  
H -0.443387 -2.846054 2.724662  
O 4.585141 0.558141 -1.072984

H 5.313800 0.901776 -1.614439  
H 4.126652 1.312996 -0.667710

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**TMZ Cat1 2w**

C -1.098706 -0.122541 -0.079259  
C -1.545912 -1.381229 0.395118  
C 0.337504 0.265285 -0.129740  
C 0.493257 -2.716317 0.320129  
C 0.929649 -1.864115 -0.892862  
O 1.251093 -3.624070 0.674498  
N 1.278434 -0.544508 -0.495514  
N -0.655066 -2.363545 0.932930  
C -2.919286 -1.665859 0.402631  
C -3.849081 -0.744639 -0.067074  
H -4.906901 -0.985951 -0.065423  
C -3.408241 0.490033 -0.552222  
C -2.052979 0.800388 -0.548908  
H -1.723948 1.764449 -0.920179  
H -3.269198 -2.624332 0.770519  
O 2.101213 -2.522040 -1.335181  
C 0.732145 1.652972 0.222168  
C 0.090195 2.347884 1.261654  
C 1.790291 2.275175 -0.467708  
C 0.511467 3.630537 1.617991  
H -0.724984 1.881462 1.807343  
C 2.195288 3.564115 -0.121596  
C 1.560367 4.242128 0.926959  
H 0.016673 4.152526 2.431876  
H 2.992757 4.047644 -0.679429  
H 1.875767 5.246607 1.194621  
H 0.201918 -1.909658 -1.712793  
Cl -4.559912 1.648199 -1.158780  
H 2.833129 -1.898896 -1.356059  
H 2.310338 -3.228295 -0.703238  
H 2.264905 1.754234 -1.293999  
C -1.063839 -3.158383 2.110969  
H -1.625126 -4.048630 1.810392  
H -0.164654 -3.475944 2.639085  
H -1.675942 -2.531610 2.760116  
O 4.274715 -1.278917 -1.361545  
H 4.829388 -1.216858 -2.154087  
H 4.471777 -0.488560 -0.796652  
O 4.828521 0.908916 0.166060  
H 5.510041 0.906601 0.856528  
H 4.081925 1.428487 0.508574

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**TMZ Cat2 0w**

C -0.175968 0.517429 -0.115354  
C -1.470000 0.790805 0.383668  
C 0.353609 -0.866921 -0.310207  
C -2.531770 -1.328052 0.051482  
C -1.720322 -1.550911 -1.217004  
O -3.355024 -2.263571 0.422755  
N -0.365214 -1.819960 -0.814704  
N -2.363724 -0.264817 0.799309  
C -1.913071 2.109597 0.533946

C -1.097704 3.174797 0.166889  
H -1.451116 4.195463 0.268212  
C 0.176744 2.916363 -0.348153  
C 0.635420 1.607306 -0.476512  
H 1.628349 1.423008 -0.870723  
H -2.905921 2.312089 0.922331  
O -2.279683 -2.697524 -1.825473  
C 1.756376 -1.166213 0.053023  
C 2.399876 -0.482150 1.102449  
C 2.449323 -2.187168 -0.625966  
C 3.704163 -0.816541 1.466018  
H 1.877561 0.294802 1.652986  
C 3.756759 -2.505620 -0.270195  
C 4.386538 -1.823305 0.777607  
H 4.186377 -0.291363 2.285303  
H 4.288516 -3.283142 -0.810916  
H 5.406310 -2.075203 1.054572  
H -1.822105 -0.684542 -1.888231  
Cl 1.199477 4.237146 -0.827916  
H -3.331505 -2.948223 -0.299212  
H -1.550285 -3.326841 -1.981158  
C -3.134548 -0.120368 2.062538  
H -4.116537 0.313993 1.856776  
H -3.263197 -1.104374 2.513410  
H -2.568570 0.524198 2.733454  
H 1.958689 -2.713445 -1.438087

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#### TMZ Cat2 1w

C -0.570612 -0.544479 -0.092888  
C 0.217782 -1.593063 0.431719  
C -0.054788 0.846148 -0.258579  
C 2.434387 -0.672267 0.219503  
C 1.996266 -0.007762 -1.082112  
O 3.622162 -0.529134 0.700028  
N 1.134475 1.087985 -0.709373  
N 1.555812 -1.368771 0.918667  
C -0.306259 -2.886734 0.543647  
C -1.600391 -3.165709 0.118302  
H -1.996339 -4.173072 0.191194  
C -2.382016 -2.137159 -0.418210  
C -1.878650 -0.842627 -0.513695  
H -2.496980 -0.054790 -0.928938  
H 0.303194 -3.688017 0.949228  
O 3.126358 0.484706 -1.751876  
C -0.928279 1.995504 0.071975  
C -1.912696 1.898884 1.073750  
C -0.744006 3.223833 -0.591020  
C -2.690701 3.007878 1.406797  
H -2.058781 0.966270 1.610762  
C -1.533096 4.323613 -0.265624  
C -2.506577 4.219303 0.735091  
H -3.439069 2.925481 2.189654  
H -1.393562 5.262568 -0.793573  
H -3.119918 5.079470 0.988358  
H 1.502071 -0.760124 -1.716490  
Cl -3.997249 -2.476296 -0.969031  
H 4.286727 -0.025924 0.109022  
H 3.038711 1.456041 -1.759290

C 1.966379 -1.966187 2.214883  
H 2.528655 -2.888989 2.047234  
H 2.597343 -1.255253 2.748765  
H 1.068159 -2.171138 2.794827  
H 0.011269 3.299998 -1.366263  
O 5.626903 0.651375 -0.468013  
H 5.752811 0.490821 -1.417415  
H 6.493083 0.548557 -0.040945

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#### TMZ Cat2 2w

C 0.766971 -0.521460 -0.045028  
C 0.204822 -1.695581 -0.593356  
C 0.029128 0.778223 -0.005361  
C -2.133371 -1.095716 -0.667178  
C -1.926163 -0.371633 0.653736  
O -3.247091 -1.119332 -1.310819  
N -1.222215 0.851912 0.316210  
N -1.086363 -1.683042 -1.229358  
C 0.920608 -2.899205 -0.583266  
C 2.186568 -2.963993 -0.011884  
H 2.732384 -3.901331 0.008801  
C 2.743428 -1.810008 0.549732  
C 2.049351 -0.603592 0.525740  
H 2.496183 0.282998 0.961565  
H 0.481571 -3.796478 -1.008289  
O -3.173660 -0.119687 1.233251  
C 0.751732 2.035630 -0.319689  
C 1.856941 2.047734 -1.190524  
C 0.294270 3.252840 0.219182  
C 2.489801 3.249098 -1.512882  
H 2.212885 1.124018 -1.637092  
C 0.936552 4.447588 -0.094148  
C 2.035663 4.449505 -0.961320  
H 3.335246 3.246264 -2.194852  
H 0.582562 5.379803 0.336972  
H 2.533982 5.383380 -1.205982  
H -1.329319 -1.023063 1.312845  
Cl 4.320470 -1.882319 1.285488  
H -4.038301 -0.570278 -0.922759  
H -3.027880 0.185889 2.161274  
C -1.251570 -2.334516 -2.552932  
H -1.759383 -3.296611 -2.442983  
H -1.850010 -1.687492 -3.195480  
H -0.264274 -2.476523 -2.988560  
H -0.564067 3.245736 0.882784  
O -5.198519 0.323802 -0.546351  
H -4.947543 0.526384 0.374216  
H -6.103557 -0.027204 -0.543778  
O -2.632357 0.627119 3.813193  
H -2.489798 1.552670 4.068115  
H -3.003992 0.184470 4.592821

\*\*\*\*

#### TMZ Cat3 0w

C -0.183547 0.503008 -0.102238  
C -1.515130 0.770190 0.339457  
C 0.374068 -0.843400 -0.221626

C -2.689044 -1.373017 0.058828  
C -1.785701 -1.657629 -1.159342  
O -3.555480 -2.182619 0.349313  
N -0.406793 -1.817147 -0.641362  
N -2.417769 -0.236287 0.774371  
C -1.926043 2.109324 0.436966  
C -1.084896 3.160026 0.090936  
H -1.438379 4.183985 0.158094  
C 0.214218 2.894502 -0.359803  
C 0.660820 1.584595 -0.445728  
H 1.663730 1.384055 -0.804416  
H -2.931114 2.334083 0.775869  
O -2.154547 -2.832290 -1.771237  
C 1.772472 -1.150579 0.088346  
C 2.419408 -0.504740 1.163498  
C 2.469798 -2.129130 -0.654472  
C 3.727305 -0.847049 1.496628  
H 1.887841 0.235231 1.753513  
C 3.782422 -2.451379 -0.324673  
C 4.410059 -1.816413 0.754154  
H 4.213942 -0.359750 2.336003  
H 4.321433 -3.186712 -0.914220  
H 5.433795 -2.072963 1.010842  
H -1.779801 -0.821112 -1.870130  
Cl 1.265355 4.203460 -0.812272  
H -2.892253 -3.215306 -1.245768  
H -0.071950 -2.780231 -0.643871  
C -3.300715 0.031028 1.932248  
H -4.238269 0.500324 1.617659  
H -3.535336 -0.922707 2.405356  
H -2.773698 0.675525 2.636280  
H 2.008214 -2.595956 -1.521336

\*\*\*\*

#### TMZ Cat3 1w

C 0.765559 -0.176479 0.080501  
C 1.099003 -1.488600 -0.364232  
C -0.606994 0.343018 0.121243  
C -1.018183 -2.716718 -0.200021  
C -1.385300 -1.826121 1.006394  
O -1.788605 -3.608035 -0.527398  
N -1.582230 -0.454152 0.492829  
N 0.140374 -2.413214 -0.860361  
C 2.451959 -1.862964 -0.388892  
C 3.455499 -1.000191 0.035564  
H 4.491682 -1.322551 0.023602  
C 3.123531 0.279698 0.494665  
C 1.798027 0.689250 0.506445  
H 1.547880 1.680607 0.866089  
H 2.724464 -2.855058 -0.731162  
O -2.564866 -2.271913 1.570950  
C -0.911917 1.736862 -0.222026  
C -0.196814 2.382384 -1.253416  
C -1.938794 2.433338 0.451089  
C -0.514791 3.689714 -1.611688  
H 0.583488 1.851536 -1.789694  
C -2.234042 3.747329 0.099583  
C -1.528413 4.375140 -0.933586  
H 0.027967 4.174450 -2.417553

H -3.008294 4.286492 0.637207  
H -1.765060 5.399687 -1.206122  
H -0.579259 -1.798111 1.750784  
Cl 4.371221 1.358622 1.048517  
H -2.864427 -3.029774 1.018488  
H -2.574285 -0.149869 0.464564  
C 0.489612 -3.278319 -2.008310  
H 0.973157 -4.203000 -1.677304  
H -0.431937 -3.539363 -2.528911  
H 1.150819 -2.726446 -2.677067  
H -2.481059 1.962218 1.265185  
O -4.321970 0.079853 0.846296  
H -5.111109 0.357125 0.354462  
H -4.585908 -0.676231 1.396710

\*\*\*\*

**TMZ Cat3 2w**

C -0.941843 -0.404048 -0.143559  
C -0.694843 -1.732648 0.306455  
C 0.126109 0.587895 -0.347648  
C 1.691479 -2.042278 -0.150510  
C 1.484996 -1.169905 -1.403123  
O 2.812748 -2.484970 0.096020  
N 1.256994 0.200225 -0.889802  
N 0.603595 -2.209379 0.650814  
C -1.785992 -2.592209 0.500589  
C -3.088372 -2.183607 0.235948  
H -3.914873 -2.872978 0.375374  
C -3.327939 -0.884391 -0.226022  
C -2.269631 -0.002819 -0.402663  
H -2.462509 1.001425 -0.762608  
H -1.613085 -3.604470 0.849558  
O 2.595529 -1.190887 -2.215302  
C -0.049973 1.993772 0.025268  
C -0.816990 2.337277 1.159518  
C 0.569438 3.014568 -0.726711  
C -0.944742 3.670554 1.538165  
H -1.283110 1.560442 1.757502  
C 0.420407 4.345723 -0.351866  
C -0.330950 4.675223 0.782188  
H -1.521627 3.927178 2.421525  
H 0.883514 5.127864 -0.945647  
H -0.441858 5.715722 1.073822  
H 0.596370 -1.471968 -1.969123  
Cl -4.952409 -0.370619 -0.577467  
H 3.312211 -1.648356 -1.728678  
H 2.118782 0.802954 -0.863884  
C 0.770905 -3.048740 1.857079  
H 0.651735 -4.110362 1.618775  
H 1.776428 -2.891263 2.246992  
H 0.034258 -2.746895 2.602034  
H 1.133900 2.767292 -1.620377  
O 3.634086 1.502225 -0.470394  
H 4.107251 0.896851 0.149007  
H 4.262907 1.718276 -1.176119  
O 4.582572 -0.480166 1.197977  
H 5.397325 -0.593344 1.710940  
H 4.257383 -1.369581 0.965726

\*\*\*\*

**TMZ TS1 0w**

C -1.627426 0.812377 0.138734  
C 0.426368 2.755769 -0.091673  
C -0.269838 0.396866 -0.057639  
C -1.868217 2.197962 0.291431  
C -0.872338 3.160258 0.191134  
C 0.710028 1.405500 -0.207262  
H -2.872720 2.555139 0.461405  
H -1.118188 4.210998 0.306357  
H 1.729626 1.113658 -0.415845  
N -2.762390 -0.025792 0.135209  
C -2.828714 -1.290749 -0.463558  
O -3.811518 -1.629587 -1.102465  
C 0.255010 -1.002232 -0.114798  
N -0.364838 -2.121934 -0.203437  
C -1.777024 -2.351536 -0.129697  
H -2.001494 -3.183514 -0.806088  
C 1.752665 -1.195328 -0.038851  
C 4.503265 -1.735451 0.151521  
C 2.421830 -1.848555 -1.082091  
C 2.472567 -0.824076 1.106841  
C 3.838097 -1.100016 1.204312  
C 3.791747 -2.106315 -0.992861  
H 1.862082 -2.158508 -1.959979  
H 1.962695 -0.325623 1.927712  
H 4.381366 -0.817135 2.102319  
H 4.300535 -2.604050 -1.814449  
H 5.567873 -1.942116 0.224211  
Cl 1.704089 3.944110 -0.289973  
O -2.093288 -2.711170 1.218001  
H -1.419336 -3.355637 1.498955  
C -4.087260 0.573682 0.369558  
H -4.074102 1.115358 1.318430  
H -4.389974 1.246362 -0.441593  
H -4.813407 -0.233603 0.430804

\*\*\*\*

**TMZ TS1 1w**

C 0.611997 1.657895 0.176662  
C -2.122563 2.331343 -0.152034  
C -0.368735 0.623343 0.062429  
C 0.156964 2.994340 0.150108  
C -1.180672 3.340389 -0.000765  
C -1.715347 1.007024 -0.124758  
H 0.864390 3.807344 0.217869  
H -1.472875 4.385356 -0.020812  
H -2.464291 0.237745 -0.249726  
N 2.013157 1.468800 0.284340  
C 2.739257 0.382659 -0.228837  
O 3.813401 0.558992 -0.773306  
C -0.127170 -0.849949 0.102371  
N 0.972540 -1.502778 0.138363  
C 2.320754 -1.031883 0.196238  
H 2.622458 -1.080036 1.258724  
C -1.329261 -1.767622 0.103625  
C -3.459755 -3.595507 0.141601  
C -2.159752 -1.865068 1.229171

C -1.569974 -2.597491 -0.998507  
C -2.635445 -3.501134 -0.982925  
C -3.215714 -2.779053 1.249946  
H -1.976530 -1.231177 2.093653  
H -0.916863 -2.537097 -1.865007  
H -2.816152 -4.135219 -1.847064  
H -3.846464 -2.852789 2.132080  
H -4.285305 -4.302225 0.155963  
Cl -3.817391 2.724552 -0.380414  
O 3.116891 -1.935204 -0.555126  
H 2.675783 -2.799016 -0.477925  
O 5.874767 -1.602350 0.286553  
H 6.103760 -0.751330 -0.116260  
H 4.989615 -1.790762 -0.080414  
C 2.859847 2.649025 0.541252  
H 2.922121 3.318168 -0.324595  
H 2.463998 3.189818 1.403709  
H 3.865068 2.300310 0.769512

\*\*\*\*

**TMZ TS1 2w**

C -0.389539 1.782376 -0.254354  
C 2.375754 2.264069 0.148971  
C 0.525754 0.685407 -0.201136  
C 0.143188 3.082664 -0.120164  
C 1.496989 3.335574 0.069648  
C 1.890192 0.972410 0.021526  
H -0.511135 3.941258 -0.132946  
H 1.849469 4.356787 0.171955  
H 2.588916 0.150939 0.093281  
N -1.800329 1.690893 -0.395979  
C -2.603891 0.601678 -0.050609  
O -3.706569 0.772145 0.443033  
C 0.203935 -0.762272 -0.360945  
N -0.923115 -1.337647 -0.541622  
C -2.235556 -0.787703 -0.588823  
H -2.541768 -0.751782 -1.648539  
C 1.341247 -1.756691 -0.305261  
C 3.350259 -3.708406 -0.196943  
C 2.188337 -1.958463 -1.402798  
C 1.498742 -2.541283 0.844656  
C 2.505586 -3.508763 0.898823  
C 3.186493 -2.934636 -1.349805  
H 2.064755 -1.357342 -2.300839  
H 0.828489 -2.393424 1.687863  
H 2.624118 -4.111006 1.795932  
H 3.834030 -3.090206 -2.208927  
H 4.129895 -4.464582 -0.154713  
Cl 4.088364 2.536755 0.414538  
O -3.084922 -1.716562 0.098942  
H -2.706006 -2.593868 -0.093054  
O -5.845872 -1.242652 -0.740569  
H -6.034654 -0.367585 -0.369717  
H -4.964778 -1.452873 -0.378531  
O -1.848159 -1.215896 2.674808  
H -2.375302 -0.805163 3.375802  
H -2.484938 -1.438283 1.968221  
C -2.567675 2.943057 -0.541789  
H -2.589393 3.529101 0.383925

H -2.132571 3.536021 -1.349098  
H -3.591914 2.684068 -0.800246

\*\*\*\*

**TMZ TS2 0w**

C -0.246774 0.405008 -0.011345  
C -1.582012 0.654885 -0.392907  
C 0.376391 -0.946882 0.188258  
C -2.542830 -1.510901 -0.065957  
C -1.590994 -2.111618 0.899340  
O -3.454164 -2.405801 -0.318313  
N -0.210361 -1.959270 0.740088  
N -2.452293 -0.409074 -0.804243  
C -2.090767 1.958537 -0.419566  
C -1.300197 3.048715 -0.069406  
H -1.700342 4.056684 -0.092675  
C 0.016240 2.811035 0.323900  
C 0.533555 1.521742 0.355044  
H 1.557039 1.369937 0.676316  
H -3.122420 2.124464 -0.713281  
O -2.024483 -2.002754 2.252137  
C 1.835486 -1.095812 -0.107666  
C 2.626343 -1.953308 0.677495  
C 2.433129 -0.445730 -1.200801  
C 3.977185 -2.137923 0.388527  
H 2.161442 -2.471263 1.510192  
C 3.783820 -0.642988 -1.499395  
C 4.562845 -1.484703 -0.702485  
H 4.576258 -2.794376 1.014878  
H 4.224760 -0.138100 -2.355327  
H 5.615537 -1.633250 -0.929281  
Cl 1.037395 4.161649 0.790310  
H -2.057191 -2.889205 2.640341  
H -2.676754 -3.107124 0.286466  
H 1.838106 0.208950 -1.832242  
C -3.300614 -0.238910 -1.994658  
H -2.755503 0.351931 -2.735075  
H -3.531992 -1.228681 -2.391690  
H -4.241761 0.261973 -1.745678

\*\*\*\*

**TMZ TS2 1w**

C 0.166949 0.564758 0.083177  
C -1.016936 1.032112 0.689244  
C 0.452005 -0.888432 -0.051791  
C -2.578406 -0.818946 0.437590  
C -1.799397 -1.533958 -0.547812  
O -3.837902 -0.942068 0.496265  
N -0.447623 -1.751194 -0.389663  
N -1.952032 0.120785 1.279579  
C -1.264811 2.414043 0.733811  
C -0.363248 3.330565 0.195090  
H -0.565478 4.395504 0.246566  
C 0.795612 2.858584 -0.417748  
C 1.060988 1.495166 -0.474941  
H 1.968932 1.142423 -0.951465  
H -2.169544 2.789209 1.197922  
O -2.448707 -2.741968 -1.000399

C 1.849474 -1.380901 0.111342  
C 2.741847 -0.768300 1.008874  
C 2.290340 -2.508963 -0.604624  
C 4.034087 -1.268347 1.186340  
H 2.419746 0.094618 1.584922  
C 3.582681 -3.001951 -0.433762  
C 4.461794 -2.384664 0.463775  
H 4.704677 -0.785082 1.892559  
H 3.907829 -3.868603 -1.004346  
H 5.469300 -2.770444 0.597097  
H -2.790753 -0.807486 -1.710272  
Cl 1.937280 3.997345 -1.120261  
O -3.868339 -0.873446 -1.997047  
H -4.166583 -0.973181 -0.978875  
H -3.903226 -1.789052 -2.343382  
H -1.896520 -3.476364 -0.680296  
H 1.603964 -2.988525 -1.295370  
C -2.813163 0.639401 2.349328  
H -3.621100 1.286250 1.983856  
H -3.271352 -0.204761 2.866150  
H -2.185378 1.192370 3.052022

\*\*\*\*

**TMZ TS2 2w**

C 0.492737 0.580007 0.166255  
C -0.601727 1.168508 0.830576  
C 0.613403 -0.896608 0.028157  
C -2.335857 -0.553831 0.773642  
C -1.722826 -1.266028 -0.323185  
O -3.548462 -0.709802 1.103242  
N -0.397118 -1.651319 -0.253207  
N -1.569931 0.361510 1.507976  
C -0.717902 2.567452 0.863840  
C 0.230574 3.388208 0.255825  
H 0.133339 4.468225 0.297179  
C 1.301976 2.797874 -0.411997  
C 1.435440 1.414797 -0.459820  
H 2.277184 0.972101 -0.981025  
H -1.554789 3.029254 1.376217  
O -2.555642 -2.317097 -0.819793  
C 1.956845 -1.538592 0.097267  
C 2.975555 -1.023609 0.918445  
C 2.217973 -2.713724 -0.631780  
C 4.215421 -1.661389 1.008023  
H 2.793672 -0.127410 1.505297  
C 3.457633 -3.344941 -0.548326  
C 4.464205 -2.822675 0.272804  
H 4.985222 -1.250100 1.656505  
H 3.641873 -4.246810 -1.127437  
H 5.430360 -3.316733 0.338150  
H -2.354415 -0.356493 -1.651388  
Cl 2.502556 3.814986 -1.200677  
O -3.099321 -0.161434 -2.390534  
H -4.450145 -0.936058 -0.086634  
H -2.398611 -3.115530 -0.284016  
O -4.980257 -0.786767 -0.980159  
H -4.107990 -0.473173 -1.756458  
H -2.954469 -0.853138 -3.061555  
H -5.585072 -0.041567 -0.826382

C -2.223223 0.929755 2.690441  
H -3.019458 1.644960 2.442935  
H -2.672176 0.120064 3.266649  
H -1.461841 1.426698 3.296338  
H 1.431301 -3.120825 -1.259290

\*\*\*\*

**TMZ TS4 0w**

C -0.273511 0.465102 -0.086356  
C -1.642318 0.499593 0.313649  
C 0.480906 -0.796387 -0.207424  
C -2.500420 -1.839372 0.000750  
C -1.527762 -1.980694 -1.192040  
O -3.309357 -2.683092 0.323823  
N -0.153541 -1.848738 -0.604490  
N -2.379315 -0.634441 0.728422  
C -2.271429 1.760163 0.379857  
C -1.608950 2.937424 0.057651  
H -2.129361 3.888650 0.105063  
C -0.272199 2.884301 -0.344923  
C 0.387077 1.667014 -0.411357  
H 1.422704 1.634180 -0.730389  
H -3.313352 1.813901 0.674555  
O -1.348357 -3.202240 -1.733258  
C 1.925486 -0.891846 0.106964  
C 2.481256 -0.162039 1.172473  
C 2.748280 -1.755982 -0.636964  
C 3.831987 -0.302524 1.491716  
H 1.852303 0.497790 1.762641  
C 4.100228 -1.883565 -0.322064  
C 4.644430 -1.159611 0.743760  
H 4.248986 0.256640 2.324761  
H 4.729313 -2.545992 -0.910123  
H 5.698029 -1.262219 0.989405  
Cl 0.572826 4.360911 -0.770681  
H -0.098596 -2.957702 -1.052940  
H -1.723158 -1.146971 -1.900399  
H 2.328245 -2.313273 -1.469265  
C -3.340431 -0.473749 1.830829  
H -4.329796 -0.160417 1.475159  
H -3.454659 -1.441301 2.320701  
H -2.952772 0.259184 2.541244

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**TMZ TS4 1w**

C -0.676250 -0.331709 -0.094915  
C -0.637054 -1.669131 0.388690  
C 0.530448 0.512714 -0.166698  
C 1.773470 -2.287167 0.224344  
C 1.853467 -1.408107 -1.063265  
O 2.696269 -2.955798 0.635131  
N 1.655245 0.003312 -0.550007  
N 0.532344 -2.272768 0.891994  
C -1.849427 -2.387753 0.441870  
C -3.049951 -1.834280 0.017840  
H -3.964430 -2.417594 0.054344  
C -3.069815 -0.524697 -0.472045  
C -1.902082 0.219937 -0.519593

H -1.926304 1.236501 -0.896118  
H -1.843302 -3.409389 0.805017  
O 3.005695 -1.499557 -1.735185  
C 0.471317 1.951672 0.188765  
C -0.344802 2.394795 1.244985  
C 1.264494 2.884767 -0.502983  
C -0.356616 3.741259 1.608461  
H -0.952513 1.682312 1.794721  
C 1.238552 4.231541 -0.145339  
C 0.431552 4.662296 0.912535  
H -0.979849 4.070124 2.435430  
H 1.847577 4.945095 -0.693184  
H 0.416067 5.712261 1.192257  
H 0.971357 -1.645739 -1.687525  
Cl -4.578156 0.178097 -1.024563  
H 3.747281 -0.634369 -1.312544  
H 2.669028 0.512135 -0.565792  
O 4.090217 0.416802 -0.768462  
H 4.522423 0.996793 -1.412756  
H 1.887252 2.555162 -1.329066  
C 0.418453 -3.188490 2.037400  
H 0.206438 -4.217470 1.721550  
H 1.374293 -3.189335 2.561965  
H -0.371760 -2.835391 2.703185

O 3.491443 1.520807 0.093900  
H 3.773021 2.331184 -0.356172  
H 4.239657 0.654276 -0.208898  
H 1.135443 2.762603 -1.455457  
C 0.627013 -3.066204 2.063212  
H 0.568192 -4.123440 1.777487  
H 1.575450 -2.908774 2.577652  
H -0.202336 -2.815295 2.727234

\*\*\*\*

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**TMZ TS4 2w**

C -0.883070 -0.435635 -0.105905  
C -0.656007 -1.747055 0.397525  
C 0.190923 0.572725 -0.184724  
C 1.809356 -2.010007 0.213794  
C 1.736831 -1.148518 -1.079263  
O 2.837633 -2.510165 0.627772  
N 1.386249 0.232915 -0.553499  
N 0.593741 -2.178274 0.890690  
C -1.754636 -2.626170 0.478830  
C -3.024953 -2.250948 0.062333  
H -3.849505 -2.954377 0.119659  
C -3.231122 -0.965114 -0.447223  
C -2.178640 -0.066466 -0.521174  
H -2.347335 0.931565 -0.910051  
H -1.602568 -3.630937 0.857324  
O 2.834768 -1.143958 -1.832343  
C -0.085918 1.990190 0.148551  
C -0.921653 2.326199 1.228414  
C 0.509019 3.016934 -0.605737  
C -1.141699 3.663241 1.557172  
H -1.379611 1.540650 1.822394  
C 0.272681 4.352490 -0.283715  
C -0.547888 4.678124 0.800540  
H -1.775949 3.912660 2.403321  
H 0.726771 5.138871 -0.880223  
H -0.727103 5.719782 1.053131  
H 0.857341 -1.476302 -1.659456  
Cl -4.827927 -0.488174 -0.990328  
H 3.835131 -0.849940 -1.257817  
H 2.277079 0.916993 -0.373163  
O 4.805779 -0.361930 -0.658840  
H 5.032738 -0.973795 0.058593

XYZ coordinates for Table S7

LOR 1ax 0w

C 0.833215 -0.169303 -0.096316  
 C -0.338282 0.755105 -0.098736  
 C 2.114951 0.234293 -0.546419  
 C 1.903460 2.749837 -0.531758  
 C 0.646349 -1.510408 0.296332  
 H -0.332410 -1.829555 0.637491  
 C 1.689827 -2.422591 0.245698  
 C 2.949035 -2.034050 -0.224564  
 C 3.150967 -0.716792 -0.611881  
 H 4.131356 -0.407221 -0.965450  
 H 3.760525 -2.752571 -0.275846  
 N 2.391072 1.532810 -0.992501  
 C -1.658791 0.163653 -0.502577  
 C -1.779237 -0.411330 -1.778815  
 C -2.800881 0.194643 0.314591  
 C -2.996256 -0.906518 -2.243071  
 C -4.022877 -0.311914 -0.135806  
 C -4.121853 -0.854379 -1.417035  
 H -3.064503 -1.330272 -3.240943  
 H -4.885632 -0.280254 0.521697  
 H -5.076776 -1.240697 -1.762838  
 O 2.297391 3.798530 -1.009861  
 Cl 1.428817 -4.079048 0.760517  
 C 0.879540 2.681018 0.616981  
 N -0.329338 2.010691 0.163098  
 H -0.901067 -0.451095 -2.418313  
 H 3.188906 1.642546 -1.611129  
 O 1.455077 2.172328 1.811711  
 H 1.567058 1.209613 1.754153  
 H 0.622801 3.712857 0.852236  
 Cl -2.732179 0.814794 1.955966

\*\*\*\*

LOR 1eq 0w

C 0.888457 -0.192100 0.058465  
 C 2.132389 0.317202 0.499605  
 C -0.355273 0.630772 0.073329  
 C 1.698747 2.778286 0.481259  
 C 0.752671 2.570732 -0.711987  
 O 1.904537 3.881366 0.964925  
 N -0.428439 1.876103 -0.221864  
 N 2.278198 1.634181 0.977923  
 C 3.254355 -0.527723 0.540080  
 C 3.169722 -1.853595 0.135007  
 H 4.044133 -2.495345 0.164095  
 C 1.944730 -2.348836 -0.323538  
 C 0.818768 -1.537719 -0.349762  
 H -0.130602 -1.942440 -0.683536  
 H 4.205550 -0.131306 0.886530  
 O 0.432950 3.797277 -1.286846  
 C -1.620733 -0.049182 0.508311  
 C -1.685530 -0.601451 1.798426  
 C -2.767581 -0.130550 -0.298929  
 C -2.854766 -1.183275 2.284775  
 H -0.802192 -0.555038 2.430464

C -3.942005 -0.721774 0.174476  
 C -3.987261 -1.240457 1.468530  
 H -2.881068 -1.588660 3.292266  
 H -4.809731 -0.774130 -0.475161  
 H -4.905474 -1.693730 1.832130  
 H 2.989604 1.802542 1.682180  
 H 1.257292 1.971746 -1.484656  
 Cl 1.830683 -4.016088 -0.857775  
 H 0.503060 4.476241 -0.589162  
 Cl -2.760032 0.455324 -1.954017

\*\*\*\*

LOR 1eq 1w

C -0.152558 0.878172 0.248940  
 C -1.247641 1.521599 0.871478  
 C 0.050554 -0.597101 0.323558  
 C -2.783851 -0.396774 1.300816  
 C -2.245412 -1.068676 0.029875  
 O -3.645215 -0.922872 1.991495  
 N -0.877294 -1.480993 0.272444  
 N -2.217175 0.812951 1.610252  
 C -1.349594 2.921686 0.826956  
 C -0.399829 3.689546 0.165662  
 H -0.492293 4.770043 0.130814  
 C 0.671275 3.051051 -0.467549  
 C 0.801729 1.670132 -0.417783  
 H 1.650057 1.190604 -0.894033  
 H -2.192929 3.408683 1.310068  
 O -3.059397 -2.168381 -0.283259  
 C 1.456341 -1.087594 0.508866  
 C 2.176303 -0.671595 1.641362  
 C 2.084618 -1.978293 -0.377771  
 C 3.459669 -1.146382 1.904869  
 H 1.706819 0.026130 2.330228  
 C 3.375664 -2.451787 -0.129115  
 C 4.058997 -2.042228 1.015851  
 H 3.987191 -0.819017 2.796242  
 H 3.836641 -3.133738 -0.836329  
 H 5.060523 -2.418711 1.205397  
 H -2.668073 1.298139 2.379481  
 H -2.301659 -0.368276 -0.816219  
 Cl 1.866698 4.008881 -1.321930  
 H -3.548197 -2.406434 0.530497  
 Cl 1.303061 -2.489902 -1.864447  
 O -4.369594 -1.059230 -2.541156  
 H -4.046506 -1.634683 -1.819324  
 H -4.360138 -1.605746 -3.340024

\*\*\*\*

LOR 1eq 2w

C -0.828639 0.713033 -0.260485  
 C -0.699978 1.971468 -0.895024  
 C 0.267457 -0.293789 -0.256038  
 C 1.771945 2.152897 -1.186534  
 C 1.948781 1.339635 0.103528  
 O 2.730067 2.564572 -1.822994  
 N 1.518524 -0.024473 -0.145967  
 N 0.472437 2.360291 -1.573582

C -1.797347 2.847690 -0.927143  
 C -3.004625 2.509034 -0.330248  
 H -3.842767 3.197677 -0.354725  
 C -3.123938 1.273731 0.314972  
 C -2.059718 0.383634 0.339294  
 H -2.173473 -0.580597 0.822586  
 H -1.692890 3.811342 -1.419148  
 O 3.298159 1.374259 0.486586  
 C -0.114312 -1.733008 -0.425812  
 C -0.788499 -2.122714 -1.595150  
 C 0.202392 -2.727523 0.514355  
 C -1.106322 -3.456817 -1.840126  
 H -1.047152 -1.362330 -2.327633  
 C -0.121697 -4.066185 0.283578  
 C -0.768381 -4.430670 -0.897129  
 H -1.612223 -3.733746 -2.760491  
 H 0.133872 -4.811286 1.029834  
 H -1.010513 -5.474962 -1.074143  
 H 0.370463 2.999803 -2.355426  
 H 1.363321 1.791235 0.916750  
 Cl -4.637474 0.843286 1.087917  
 H 3.818345 1.612270 -0.308383  
 Cl 0.963689 -2.325224 2.045928  
 O 2.850916 3.264692 2.549734  
 H 3.285211 2.629736 1.946792  
 H 3.328272 3.208925 3.389810  
 O 3.811769 -1.882044 -0.712105  
 H 4.352451 -1.880134 0.091315  
 H 3.054705 -1.300039 -0.497662

\*\*\*\*

LOR An1 0w

C 0.900310 -0.174831 0.203740  
 C 2.106766 0.514714 0.495484  
 C -0.409111 0.485896 0.242530  
 C 1.523833 2.906284 0.422762  
 C 0.227072 2.760536 -0.183817  
 O 2.114607 4.009746 0.477047  
 N -0.610829 1.768347 -0.066523  
 N 2.061997 1.799740 1.118682  
 C 3.346580 -0.098532 0.299458  
 C 3.454349 -1.430303 -0.120873  
 H 4.420680 -1.911004 -0.231245  
 C 2.270039 -2.113860 -0.386061  
 C 1.026180 -1.511023 -0.252550  
 H 0.131418 -2.070683 -0.501222  
 H 4.252345 0.462326 0.525014  
 O -0.269718 3.948020 -0.721135  
 C -1.621407 -0.329473 0.468707  
 C -1.635108 -1.256007 1.543302  
 C -2.828987 -0.250351 -0.269782  
 C -2.748319 -2.018903 1.877674  
 H -0.729966 -1.343018 2.138965  
 C -3.961237 -0.996193 0.067931  
 C -3.934211 -1.884003 1.144787  
 H -2.698008 -2.704060 2.721753  
 H -4.857595 -0.889536 -0.536621  
 H -4.820199 -2.461414 1.398372  
 Cl 2.356486 -3.803099 -0.936952

H 0.423670 4.608475 -0.526504  
Cl -2.962360 0.742429 -1.723317  
H 2.959740 2.077876 1.503903

\*\*\*\*

LOR An1 1w

C 0.041882 -0.903507 0.304303  
C 1.259611 -1.486291 0.735769  
C -0.198256 0.548431 0.364443  
C 2.846258 0.383009 0.859404  
C 2.046879 1.367259 0.209272  
O 4.088745 0.520652 1.034658  
N 0.737499 1.471953 0.203670  
N 2.194248 -0.709965 1.484876  
C 1.507572 -2.847230 0.533770  
C 0.548932 -3.692755 -0.036127  
H 0.735888 -4.754964 -0.154632  
C -0.653794 -3.122139 -0.444086  
C -0.904522 -1.762712 -0.300812  
H -1.842937 -1.351195 -0.655503  
H 2.456312 -3.265544 0.865332  
O 2.758066 2.485324 -0.243116  
C -1.594460 1.038722 0.459701  
C -2.446533 0.489263 1.448776  
C -2.166088 2.062003 -0.333747  
C -3.749158 0.930471 1.657689  
H -2.039776 -0.297499 2.078971  
C -3.467475 2.526173 -0.123926  
C -4.267691 1.967964 0.873971  
H -4.353476 0.477272 2.440795  
H -3.852719 3.314981 -0.763709  
H -5.279765 2.334606 1.028408  
Cl -1.893082 -4.156605 -1.185087  
H 3.615059 2.458258 0.222380  
Cl -1.296480 2.771103 -1.694076  
H 2.908105 -1.283117 1.925191  
O 5.487759 1.145622 -1.392548  
H 4.697663 1.555398 -1.780197  
H 5.160491 0.826677 -0.523431

\*\*\*\*

LOR An1 2w

C -0.039298 0.619412 0.147517  
C -1.430566 0.573136 0.400099  
C 0.806349 -0.589656 0.188301  
C -2.023914 -1.789505 0.179741  
C -0.811480 -2.251734 -0.392773  
O -3.086299 -2.491171 0.132412  
N 0.405318 -1.794407 -0.181221  
N -2.005802 -0.611506 0.958757  
C -2.233590 1.702866 0.215653  
C -1.679105 2.931290 -0.161772  
H -2.299669 3.815375 -0.264157  
C -0.307622 2.981978 -0.397305  
C 0.499939 1.857960 -0.268131  
H 1.559996 1.930276 -0.485009  
H -3.303521 1.635614 0.405904  
O -0.902828 -3.492341 -1.025064

C 2.246071 -0.440816 0.510366  
C 2.614229 0.311091 1.652905  
C 3.319058 -1.024060 -0.204919  
C 3.932490 0.455883 2.072597  
H 1.815438 0.770946 2.229072  
C 4.646296 -0.899314 0.214296  
C 4.963794 -0.162821 1.356475  
H 4.153689 1.037282 2.965220  
H 5.428619 -1.368952 -0.374986  
H 5.999886 -0.070333 1.673500  
Cl 0.428997 4.521478 -0.890727  
H -1.826731 -3.772336 -0.881502  
Cl 3.060147 -1.888524 -1.720083  
H -2.926992 -0.443984 1.351830  
O -5.479200 -1.626377 0.947083  
H -6.123342 -2.304569 0.699241  
H -4.585549 -1.983467 0.665582  
O -5.778538 0.906063 -0.214754  
H -5.732562 0.020477 0.216579  
H -5.312302 0.791183 -1.055980

\*\*\*\*

LOR An2 0w

C 0.840902 -0.272348 0.048929  
C 2.148282 0.044714 0.498464  
C -0.248606 0.751721 0.039190  
C 2.127966 2.585942 0.424639  
C 1.204845 2.545227 -0.857315  
O 2.617842 3.570601 0.947325  
N -0.132335 1.988331 -0.255604  
N 2.494246 1.316245 0.948141  
C 3.111320 -0.983945 0.577233  
C 2.815449 -2.291051 0.210085  
H 3.571737 -3.067717 0.270520  
C 1.529997 -2.586141 -0.249130  
C 0.555741 -1.599863 -0.317321  
H -0.445350 -1.851820 -0.652486  
H 4.113059 -0.740161 0.925260  
O 1.079256 3.642133 -1.509098  
C -1.605456 0.281843 0.505025  
C -1.781208 -0.074752 1.853851  
C -2.739143 0.229943 -0.321279  
C -3.026397 -0.435920 2.366604  
H -0.912623 -0.047604 2.507735  
C -3.994164 -0.135069 0.174357  
C -4.140900 -0.463094 1.522886  
H -3.126976 -0.692156 3.418737  
H -4.844797 -0.162647 -0.500055  
H -5.119686 -0.741551 1.906486  
Cl 1.141454 -4.244342 -0.736747  
Cl -2.614873 0.588273 -2.040044  
H 3.300918 1.373533 1.562613  
H 1.609913 1.666159 -1.444227

\*\*\*\*

LOR An2 1w

C 0.030832 0.947203 -0.192892  
C 0.940101 1.855928 -0.790219

C 0.180074 -0.528817 -0.372914  
C 2.910014 0.347507 -1.327582  
C 2.604471 -0.497154 -0.039745  
O 3.847220 0.207719 -2.089806  
N 1.276626 -1.183625 -0.391057  
N 2.022223 1.428804 -1.557720  
C 0.697321 3.240762 -0.676309  
C -0.398162 3.732687 0.022494  
H -0.565887 4.801977 0.106582  
C -1.274441 2.827801 0.626673  
C -1.073282 1.459480 0.511917  
H -1.778482 0.769159 0.963538  
H 1.393718 3.936990 -1.138954  
O 3.547429 -1.313786 0.326052  
C -1.089053 -1.299137 -0.635727  
C -1.829947 -1.020040 -1.797347  
C -1.559386 -2.329789 0.194648  
C -2.969180 -1.747525 -2.138936  
H -1.483825 -0.219823 -2.447310  
C -2.704106 -3.063972 -0.131136  
C -3.407086 -2.777709 -1.301845  
H -3.509425 -1.513772 -3.053206  
H -3.036369 -3.852170 0.537620  
H -4.293506 -3.355594 -1.552706  
Cl -2.663466 3.440379 1.535611  
Cl -0.747524 -2.713725 1.703936  
H 2.396435 2.096526 -2.224783  
H 2.325278 0.281014 0.729001  
O 3.844601 -1.590791 2.976493  
H 3.748988 -1.557353 1.969742  
H 3.434929 -0.764817 3.271228

\*\*\*\*

LOR An2 2w

C 0.590247 -0.905787 -0.203322  
C 0.008775 -2.076959 -0.747872  
C -0.104267 0.414146 -0.272738  
C -2.407927 -1.375642 -1.015719  
C -2.288301 -0.500138 0.276269  
O -3.412618 -1.551595 -1.684010  
N -1.357053 0.623142 -0.136577  
N -1.237088 -2.067269 -1.377911  
C 0.744556 -3.278967 -0.733987  
C 2.020135 -3.343658 -0.187566  
H 2.571004 -4.278941 -0.178304  
C 2.577788 -2.186775 0.362483  
C 1.882668 -0.986191 0.346823  
H 2.339534 -0.091834 0.757690  
H 0.294826 -4.176563 -1.152746  
O -3.435202 -0.084849 0.770593  
C 0.757203 1.607834 -0.601245  
C 1.329957 1.705672 -1.880356  
C 0.988120 2.665903 0.290947  
C 2.076089 2.817451 -2.269026  
H 1.164572 0.891406 -2.581814  
C 1.738713 3.785165 -0.081073  
C 2.278831 3.863953 -1.364937  
H 2.492650 2.868425 -3.271944  
H 1.894820 4.583628 0.637812

H 2.857090 4.738721 -1.652509  
Cl 4.193718 -2.257460 1.074974  
Cl 0.372059 2.604998 1.936399  
H -1.411337 -2.800553 -2.057929  
H -1.702985 -1.132716 0.991026  
O -3.523178 -0.360588 3.430774  
H -3.546579 -0.307336 2.424552  
H -3.360591 0.556912 3.693446  
O -5.413247 0.697725 -0.997453  
H -5.199785 -0.043189 -1.586481  
H -4.733990 0.551186 -0.286052

\*\*\*\*

LOR An3 0w

C 0.904686 -0.190656 0.052163  
C 2.197546 0.325716 0.422586  
C -0.293799 0.668218 0.042711  
C 1.841491 2.671717 0.518588  
C 0.862579 2.582450 -0.700052  
O 1.964585 3.802860 1.034379  
N -0.340646 1.921835 -0.245196  
N 2.489834 1.568696 0.890796  
C 3.279523 -0.611613 0.413593  
C 3.122699 -1.942815 0.082310  
H 3.972374 -2.620164 0.084555  
C 1.841744 -2.417492 -0.248618  
C 0.755419 -1.565924 -0.248664  
H -0.228486 -1.951156 -0.498660  
H 4.254708 -0.227027 0.699562  
O 0.588276 3.877726 -1.165112  
C -1.599104 0.054213 0.482659  
C -1.723542 -0.388150 1.810803  
C -2.727240 -0.069532 -0.341516  
C -2.919749 -0.904269 2.306865  
H -0.853800 -0.309041 2.457820  
C -3.932888 -0.592575 0.136547  
C -4.031323 -1.005256 1.465283  
H -2.983447 -1.225967 3.343501  
H -4.781415 -0.675090 -0.535841  
H -4.971244 -1.408197 1.835416  
H 1.323350 2.006977 -1.517614  
Cl 1.630119 -4.131403 -0.669864  
H 0.903929 4.446269 -0.424857  
Cl -2.663733 0.390274 -2.041239

\*\*\*\*

LOR An3 1w

C -0.455483 0.545008 -0.160897  
C -1.879517 0.551784 0.020715  
C 0.329533 -0.703342 -0.074130  
C -2.441855 -1.766489 -0.055010  
C -1.325082 -2.020855 -1.111930  
O -3.084023 -2.768224 0.327467  
N -0.046321 -1.874514 -0.447954  
N -2.671058 -0.514900 0.347482  
C -2.526966 1.822880 -0.026578  
C -1.843042 3.003134 -0.248596  
H -2.371856 3.951348 -0.285071

C -0.449418 2.964369 -0.415235  
C 0.233245 1.765561 -0.354574  
H 1.312883 1.754715 -0.467996  
H -3.601696 1.834273 0.131158  
O -1.476977 -3.308901 -1.644911  
C 1.685952 -0.629633 0.579679  
C 1.763113 -0.289016 1.940702  
C 2.889790 -0.921646 -0.078500  
C 2.977038 -0.266753 2.625904  
H 0.839621 -0.049139 2.461329  
C 4.117152 -0.895244 0.590962  
C 4.160047 -0.573458 1.947628  
H 2.998655 -0.010467 3.682199  
H 5.027038 -1.123025 0.044065  
H 5.115451 -0.557446 2.466816  
H -1.407957 -1.291249 -1.932271  
Cl 0.436430 4.476167 -0.700355  
H -2.098888 -3.741416 -1.016696  
Cl 2.915355 -1.292557 -1.800450  
O -5.131030 -0.408970 1.802268  
H -5.366480 -1.346324 1.877254  
H -4.276262 -0.445778 1.296773

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LOR An3 2w

C 0.026811 0.722594 -0.248282  
C -1.362070 1.070965 -0.192557  
C 0.474830 -0.684120 -0.175173  
C -2.447311 -1.022296 -0.467742  
C -1.334506 -1.485702 -1.449575  
O -3.334353 -1.881087 -0.210183  
N -0.133697 -1.703719 -0.667376  
N -2.415056 0.212258 0.010590  
C -1.681352 2.458913 -0.225997  
C -0.715924 3.444098 -0.322855  
H -0.996736 4.492838 -0.352591  
C 0.636798 3.073088 -0.366363  
C 1.004312 1.742777 -0.311025  
H 2.055486 1.472358 -0.328916  
H -2.731598 2.728227 -0.159543  
O -1.735349 -2.657828 -2.105904  
C 1.728428 -0.976794 0.607253  
C 1.738117 -0.710874 1.987073  
C 2.886992 -1.539461 0.051809  
C 2.838779 -1.015698 2.786307  
H 0.850963 -0.264683 2.428992  
C 4.003008 -1.842829 0.837567  
C 3.976302 -1.586334 2.208403  
H 2.808163 -0.808362 3.852918  
H 4.882631 -2.273537 0.369153  
H 4.844386 -1.827208 2.817395  
H -1.154389 -0.710414 -2.209680  
Cl 1.881361 4.330914 -0.487890  
H -2.474283 -2.993493 -1.552886  
Cl 3.007177 -1.848770 -1.678110  
O -5.647350 -1.576789 1.239507  
H -4.769846 -1.702774 0.790249  
H -6.277789 -1.520137 0.506671  
O -4.753850 1.179450 1.598817

H -5.220217 0.323614 1.680285  
H -3.952718 0.927431 1.086493

\*\*\*\*

LOR Cat1 0w

C 0.947202 -0.020080 0.067112  
C 2.033367 0.796067 0.473779  
C -0.470704 0.425834 0.094325  
C 1.023642 3.057212 0.507875  
C 0.081524 2.597893 -0.620286  
O 0.902572 4.210786 0.922217  
N -0.854074 1.630425 -0.178526  
N 1.867175 2.119797 0.972110  
C 3.336111 0.281486 0.467446  
C 3.590575 -1.015847 0.038719  
H 4.604939 -1.400690 0.030264  
C 2.527906 -1.818190 -0.392268  
C 1.225440 -1.332101 -0.364983  
H 0.409174 -1.970321 -0.683627  
H 4.161241 0.908053 0.795951  
O -0.662586 3.758768 -0.891384  
C -1.520819 -0.555181 0.471885  
C -1.332941 -1.321666 1.639042  
C -2.721580 -0.726600 -0.248402  
C -2.311673 -2.199813 2.095345  
H -0.412551 -1.203879 2.204031  
C -3.696189 -1.621507 0.194271  
C -3.495804 -2.348135 1.369203  
H -2.149733 -2.766206 3.007146  
H -4.603350 -1.749814 -0.386833  
H -4.264671 -3.036432 1.707868  
H 2.524945 2.442694 1.677892  
H 0.621349 2.332252 -1.537523  
Cl 2.835097 -3.436216 -0.953067  
Cl -3.022945 0.096060 -1.770864  
H -1.598340 3.570122 -0.789510  
H -0.407509 4.452660 -0.278970

\*\*\*\*

LOR Cat1 1w

C -1.064644 0.433458 -0.067421  
C -1.552467 1.685495 -0.515306  
C 0.368062 0.041771 -0.152290  
C 0.526552 3.017689 -0.698317  
C 1.101864 2.184678 0.464784  
O 1.231864 3.893066 -1.193815  
N 1.357123 0.844097 0.061594  
N -0.711893 2.669408 -1.102262  
C -2.924723 1.963306 -0.457206  
C -3.819516 1.035941 0.062973  
H -4.879171 1.264026 0.110648  
C -3.340486 -0.191681 0.535333  
C -1.985912 -0.494221 0.457492  
H -1.631766 -1.457617 0.806930  
H -3.293011 2.920380 -0.817246  
O 2.329642 2.813836 0.732262  
C 0.688865 -1.360720 -0.543151  
C 0.039140 -1.901153 -1.669991



C 1.642549 -2.167772 0.106808  
C 0.343486 -3.173488 -2.147187  
H -0.701473 -1.298268 -2.187469  
C 1.938629 -3.451275 -0.349578  
C 1.295319 -3.950191 -1.483783  
H -0.162927 -3.556523 -3.027711  
H 2.663011 -4.055798 0.186055  
H 1.535578 -4.948243 -1.838129  
H -1.110327 3.261548 -1.826724  
H 0.486681 2.268896 1.369662  
CI -4.448409 -1.352431 1.211341  
CI 2.455882 -1.646166 1.585389  
H 3.026761 2.154591 0.764246  
H 2.521523 3.449071 0.038532  
O 4.242820 1.155738 0.797763  
H 5.013460 1.210130 1.385830  
H 3.913076 0.237279 0.827012

\*\*\*\*

LOR Cat1 2w

C 1.372814 -0.564232 -0.043180  
C 1.692707 -1.870359 -0.487428  
C 0.036529 0.057869 -0.250808  
C -0.546884 -2.846069 -0.900045  
C -1.082592 -1.942508 0.226390  
O -1.325677 -3.596594 -1.481754  
N -1.082834 -0.578631 -0.158507  
N 0.764723 -2.692967 -1.180721  
C 2.990213 -2.370789 -0.312785  
C 3.968388 -1.613770 0.320395  
H 4.967452 -2.013693 0.458411  
C 3.649789 -0.334246 0.790103  
C 2.376086 0.188318 0.598432  
H 2.149294 1.189587 0.947583  
H 3.231631 -3.368506 -0.669915  
O -2.447957 -2.382535 0.374224  
C -0.014868 1.500289 -0.622350  
C 0.836766 1.954077 -1.648651  
C -0.899941 2.434450 -0.048778  
C 0.794089 3.268848 -2.104968  
H 1.527768 1.251867 -2.106099  
C -0.934106 3.758835 -0.484796  
C -0.093646 4.173518 -1.519238  
H 1.452054 3.584633 -2.908670  
H -1.612627 4.459243 -0.009254  
H -0.131411 5.204971 -1.857182  
H 1.131402 -3.334250 -1.879471  
H -0.589470 -2.143156 1.185356  
CI 4.860550 0.614769 1.607706  
CI -1.956192 2.016236 1.299210  
H -3.048860 -1.640734 0.280232  
H -2.651438 -2.984575 -0.361281  
O -4.103447 -0.543487 0.078309  
H -4.988668 -0.509497 0.513959  
H -3.698576 0.337868 0.149675  
O -6.567822 -0.450092 1.291380  
H -7.405107 -0.367586 0.808615  
H -6.793605 -0.475788 2.234047

\*\*\*\*

LOR Cat2 0w

C 0.931692 -0.070823 0.055962  
C 2.073312 0.664160 0.453638  
C -0.456728 0.474765 0.091328  
C 1.171946 2.929176 0.467205  
C 0.219754 2.617991 -0.668816  
O 1.148564 4.102739 1.016000  
N -0.771485 1.695554 -0.182210  
N 1.984262 2.010660 0.930846  
C 3.343044 0.077603 0.463401  
C 3.512561 -1.235759 0.041888  
H 4.498960 -1.687195 0.036076  
C 2.397408 -1.968372 -0.382645  
C 1.125575 -1.400721 -0.358592  
H 0.269622 -1.990094 -0.667073  
H 4.205340 0.653160 0.790272  
O -0.380781 3.848855 -1.003577  
C -1.558958 -0.445921 0.483635  
C -1.429673 -1.186467 1.674311  
C -2.751325 -0.578659 -0.257132  
C -2.458936 -2.002529 2.135240  
H -0.514509 -1.099354 2.253993  
C -3.777796 -1.411293 0.191818  
C -3.635726 -2.112518 1.390039  
H -2.342526 -2.550417 3.065178  
H -4.679797 -1.510099 -0.402985  
H -4.444083 -2.751762 1.732886  
H 2.622425 2.290450 1.675692  
H 0.788500 2.225534 -1.527021  
CI 2.598229 -3.604305 -0.929632  
CI -2.976075 0.216309 -1.803928  
H 0.498424 4.643975 0.492427  
H -1.347583 3.711701 -1.006417

\*\*\*\*

LOR Cat2 1w

C 0.439722 0.927522 0.047295  
C -0.302433 2.069066 0.428330  
C -0.121194 -0.451454 0.075344  
C -2.594415 1.180547 0.430209  
C -2.244556 0.257266 -0.725129  
O -3.738841 1.210733 1.009588  
N -1.341201 -0.746372 -0.217478  
N -1.650062 1.982636 0.891818  
C 0.290230 3.337097 0.443124  
C 1.612047 3.500960 0.047359  
H 2.066794 4.485874 0.046966  
C 2.350320 2.382195 -0.357833  
C 1.778837 1.113214 -0.341874  
H 2.370314 0.253650 -0.636272  
H -0.288743 4.202187 0.756187  
O -3.411918 -0.356950 -1.200033  
C 0.777390 -1.566622 0.487356  
C 1.484497 -1.451917 1.699007  
C 0.922354 -2.754202 -0.257166  
C 2.280216 -2.490508 2.175143  
H 1.388252 -0.539492 2.281588

C 1.733830 -3.791004 0.207019  
C 2.402581 -3.662876 1.425119  
H 2.802921 -2.384435 3.120748  
H 1.841676 -4.689604 -0.391375  
H 3.026138 -4.478416 1.779744  
H -1.929443 2.620032 1.636203  
H -1.794342 0.866764 -1.526249  
CI 3.999753 2.577954 -0.871951  
CI 0.166176 -2.961608 -1.826435  
H -4.491728 0.644389 0.587091  
H -3.273550 -1.317860 -1.099442  
O -5.831424 -0.040261 0.205488  
H -5.910432 -0.180007 -0.752444  
H -6.688894 0.281299 0.529273

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LOR Cat2 2w

C -1.001648 -0.821806 0.034593  
C -0.683606 -2.148802 0.407052  
C -0.015853 0.295250 0.088176  
C 1.767506 -2.042114 0.453053  
C 1.738456 -1.075220 -0.722582  
O 2.831267 -2.411891 1.061027  
N 1.233150 0.178713 -0.206593  
N 0.608399 -2.509188 0.893450  
C -1.661871 -3.149997 0.392631  
C -2.957300 -2.863615 -0.020496  
H -3.711522 -3.643052 -0.043123  
C -3.278198 -1.558966 -0.414772  
C -2.320467 -0.550316 -0.372683  
H -2.590589 0.459499 -0.660690  
H -1.404766 -4.161339 0.696890  
O 3.015977 -0.930084 -1.249289  
C -0.502298 1.633724 0.533068  
C -1.198858 1.727543 1.752327  
C -0.265543 2.820466 -0.187474  
C -1.617007 2.956100 2.257364  
H -1.396880 0.820335 2.317129  
C -0.699183 4.053157 0.304596  
C -1.364865 4.121347 1.529160  
H -2.139470 3.002767 3.207961  
H -0.519555 4.950691 -0.278026  
H -1.693629 5.085778 1.905386  
H 0.654128 -3.189336 1.650492  
H 1.079272 -1.508481 -1.492968  
CI -4.892819 -1.192436 -0.950016  
CI 0.510345 2.806595 -1.761816  
H 3.741982 -2.004608 0.748470  
H 3.350285 -0.028346 -1.061265  
O 5.170017 -1.483597 0.771001  
H 5.319504 -0.708117 0.185834  
H 5.884788 -2.120013 0.611223  
O 5.075787 0.911848 -0.709579  
H 5.090410 1.716225 -0.164460  
H 5.567259 1.129897 -1.519079

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LOR Cat3 0w

C 0.942364 -0.027628 0.064318  
C 2.021763 0.803527 0.485634  
C -0.460712 0.376137 0.119423  
C 1.045609 3.102683 0.526951  
C 0.092967 2.699834 -0.615298  
O 1.033759 4.238475 0.961211  
N -0.792852 1.628284 -0.099822  
N 1.853064 2.102568 1.003636  
C 3.323368 0.278990 0.478727  
C 3.582477 -1.010190 0.033674  
H 4.599415 -1.389070 0.024083  
C 2.528237 -1.816699 -0.419965  
C 1.228171 -1.337846 -0.391337  
H 0.418457 -1.969193 -0.738042  
H 4.147021 0.901952 0.816681  
O -0.692166 3.761389 -0.994284  
C -1.516362 -0.597459 0.450469  
C -1.285797 -1.473000 1.535959  
C -2.761817 -0.678272 -0.220462  
C -2.259020 -2.371450 1.957252  
H -0.340185 -1.417186 2.065945  
C -3.726461 -1.597239 0.188500  
C -3.479941 -2.433266 1.279737  
H -2.066038 -3.019849 2.805890  
H -4.664186 -1.658611 -0.353669  
H -4.244869 -3.137850 1.592684  
H 2.552017 2.425250 1.668804  
H 0.648916 2.286072 -1.468183  
CI 2.852353 -3.419640 -1.009015  
H -0.469045 4.522333 -0.414522  
CI -3.124053 0.296755 -1.631701  
H -1.765902 1.921582 -0.011106

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LOR Cat3 1w

C -1.086341 -0.317377 0.067732  
C -1.744212 -1.516727 0.468364  
C 0.364470 -0.138268 0.106292  
C 0.070140 -3.231724 0.432557  
C 0.759958 -2.445403 -0.697031  
O 0.546353 -4.277339 0.835234  
N 1.173730 -1.138129 -0.139771  
N -1.067079 -2.658906 0.938578  
C -3.147166 -1.546870 0.491795  
C -3.901012 -0.449353 0.099083  
H -4.985047 -0.499647 0.112452  
C -3.257263 0.721042 -0.328519  
C -1.873305 0.790408 -0.329150  
H -1.383009 1.701994 -0.650568  
H -3.652449 -2.453825 0.812568  
O 1.871707 -3.118178 -1.147893  
C 0.944942 1.177069 0.450235  
C 0.505755 1.810655 1.631276  
C 1.928186 1.821022 -0.333081  
C 1.054203 3.020796 2.042856  
H -0.255619 1.327658 2.236738  
C 2.459221 3.046447 0.066164  
C 2.032313 3.637098 1.257132  
H 0.716863 3.482818 2.965248

H 3.197177 3.535994 -0.560558  
H 2.459567 4.587969 1.561923  
H -1.568702 -3.253386 1.594007  
H 0.059635 -2.245050 -1.519573  
CI -4.197947 2.088705 -0.847805  
H 1.983024 -3.914585 -0.585048  
CI 2.446751 1.169449 -1.876349  
H 2.198318 -1.040666 0.019684  
O 3.920186 -0.862907 0.469476  
H 4.537942 -0.911182 -0.278236  
H 4.350778 -1.332966 1.201580

\*\*\*\*

LOR Cat3 2w

C 1.231266 0.559556 0.061593  
C 1.475259 1.908401 0.448681  
C -0.109224 -0.016580 -0.060831  
C -0.719059 3.036726 0.070948  
C -0.999868 2.048628 -1.075735  
O -1.517925 3.916358 0.338987  
N -1.118937 0.700350 -0.479795  
N 0.452721 2.829913 0.749473  
C 2.799615 2.333525 0.636454  
C 3.871144 1.478145 0.419101  
H 4.887880 1.831406 0.557745  
C 3.635630 0.158727 0.007035  
C 2.336644 -0.296886 -0.153837  
H 2.162147 -1.321664 -0.460555  
H 2.988604 3.357648 0.946791  
O -2.171258 2.372780 -1.720510  
C -0.346893 -1.428528 0.312481  
C 0.062391 -1.859236 1.590849  
C -0.974968 -2.359372 -0.542767  
C -0.182044 -3.159014 2.021746  
H 0.554057 -1.152759 2.253427  
C -1.196691 -3.669528 -0.120742  
C -0.812865 -4.063156 1.162413  
H 0.123586 -3.466523 3.016851  
H -1.661272 -4.375790 -0.800651  
H -0.998003 -5.084177 1.483241  
H 0.675800 3.562673 1.418396  
H -0.159944 2.023232 -1.783448  
CI 4.976285 -0.909858 -0.290992  
H -2.586638 3.109401 -1.223345  
CI -1.410687 -1.945709 -2.189402  
H -2.102845 0.325125 -0.423487  
O -3.660560 -0.270576 -0.138956  
H -4.201867 -0.393096 -0.934020  
H -4.242701 0.148399 0.536706  
O -5.205545 0.878904 1.860158  
H -5.712633 0.323768 2.473173  
H -5.657538 1.736979 1.836359

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LOR TS1 0w

C 1.835916 1.222868 -0.043389  
C -0.392800 2.928072 -0.142728  
C 0.537920 0.661783 -0.117593

C 1.977181 2.625087 -0.024992  
C 0.886780 3.479618 -0.073553  
C -0.557955 1.552503 -0.165952  
H 2.976217 3.051175 0.029264  
H 1.028266 4.555336 -0.057823  
H -1.561150 1.151049 -0.224366  
N 3.041484 0.518724 0.018279  
C 3.426970 -0.802447 0.122918  
O 4.607358 -1.053592 0.307079  
C 0.235325 -0.794757 -0.169607  
N 1.002436 -1.813942 -0.104863  
C 2.423166 -1.961851 0.046117  
H 2.564226 -2.508099 0.992853  
C -1.214441 -1.186241 -0.371552  
C -3.860221 -2.042704 -0.804362  
C -2.085094 -1.412444 0.701050  
C -1.697744 -1.400780 -1.669909  
C -3.008524 -1.824199 -1.890642  
C -3.399355 -1.838103 0.496787  
H -1.028757 -1.236891 -2.510971  
H -3.361266 -1.985669 -2.905394  
H -4.046988 -2.007286 1.351151  
H -4.882515 -2.374003 -0.964785  
CI -1.797101 3.979252 -0.204798  
H 3.863647 1.109888 0.105222  
O 2.881003 -2.750330 -1.045397  
H 2.201167 -3.432593 -1.184226  
CI -1.532895 -1.159454 2.353396

\*\*\*\*

LOR TS1 1w

C -1.466526 1.588366 -0.237722  
C 0.982993 2.851812 0.283858  
C -0.304696 0.798643 -0.069574  
C -1.364912 2.990213 -0.149835  
C -0.161353 3.629076 0.106570  
C 0.907894 1.470669 0.198729  
H -2.261342 3.591791 -0.281282  
H -0.114254 4.711126 0.170899  
H 1.809792 0.890990 0.343568  
N -2.759369 1.117926 -0.493126  
C -3.377904 -0.107201 -0.589505  
O -4.589839 -0.146880 -0.741922  
C -0.255288 -0.685240 -0.156628  
N -1.168782 -1.539423 -0.418809  
C -2.579997 -1.419300 -0.624113  
H -2.787001 -1.831643 -1.623254  
C 1.068682 -1.348989 0.153998  
C 3.444727 -2.698740 0.809042  
C 2.056295 -1.576585 -0.810133  
C 1.287603 -1.818168 1.458020  
C 2.468148 -2.485239 1.786266  
C 3.240281 -2.246729 -0.495474  
H 0.512791 -1.658078 2.204307  
H 2.621824 -2.841789 2.801009  
H 3.985702 -2.410850 -1.267064  
H 4.365865 -3.219589 1.056310  
CI 2.522640 3.625177 0.618891  
H -3.458396 1.850555 -0.579472

O -3.203228 -2.251261 0.364854  
H -2.734412 -3.103788 0.325180  
O -2.044933 -1.160152 2.761788  
H -2.652401 -0.958773 3.488652  
H -2.591157 -1.575738 2.063182  
CI 1.820205 -1.018291 -2.464610

\*\*\*\*

LOR TS1 2w

C -0.637342 1.937294 -0.353852  
C 2.021992 2.505316 0.323700  
C 0.248293 0.867045 -0.087193  
C -0.162094 3.260212 -0.292518  
C 1.151150 3.556969 0.040285  
C 1.577523 1.194027 0.258639  
H -0.847856 4.077160 -0.504567  
H 1.489867 4.586764 0.083687  
H 2.274192 0.397015 0.481600  
N -1.991619 1.824219 -0.699125  
C -2.927506 0.823651 -0.685989  
O -4.103452 1.098898 -0.893355  
C -0.100319 -0.577692 -0.149689  
N -1.216975 -1.162834 -0.368785  
C -2.542112 -0.654598 -0.531778  
H -2.946468 -1.122744 -1.440244  
C 1.011695 -1.565262 0.124720  
C 2.975548 -3.489860 0.699569  
C 1.902335 -2.000972 -0.862208  
C 1.115275 -2.116979 1.410389  
C 2.093177 -3.069337 1.698911  
C 2.880943 -2.958184 -0.587488  
H 0.417153 -1.784288 2.174911  
H 2.162317 -3.484771 2.700426  
H 3.553560 -3.280240 -1.376025  
H 3.737484 -4.233751 0.916101  
CI 3.686252 2.842454 0.763245  
H -2.446576 2.711668 -0.896239  
O -3.308544 -1.116270 0.599523  
H -3.165395 -2.079222 0.649247  
O -6.249064 -0.946400 0.234797  
H -6.431546 -0.192213 -0.346136  
H -5.287651 -0.886348 0.378758  
O -1.647358 -0.339489 2.835793  
H -2.069746 0.006232 3.636106  
H -2.374655 -0.563880 2.222503  
CI 1.796777 -1.349793 -2.495705

\*\*\*\*

LOR TS2 0w

C 0.558883 -0.489145 0.081270  
C 1.809835 -0.926340 -0.403449  
C 0.133171 0.937858 0.278872  
C 3.066147 1.162752 -0.315800  
C 2.268356 1.992752 0.607379  
O 4.057471 1.880266 -0.743687  
N 0.868350 1.939366 0.621912  
N 2.793682 -0.012096 -0.873116  
C 2.113567 -2.286534 -0.500585

C 1.196313 -3.258636 -0.110629  
H 1.435466 -4.313546 -0.190073  
C -0.032418 -2.839760 0.395257  
C -0.346686 -1.487923 0.488812  
H -1.315224 -1.198713 0.879013  
H 3.085931 -2.587491 -0.882562  
O 2.821248 2.027620 1.921189  
C -1.343859 1.218531 0.265190  
C -1.944441 1.769626 1.409854  
C -2.161251 1.007577 -0.855688  
C -3.304778 2.069446 1.445604  
H -1.314018 1.961382 2.273019  
C -3.524789 1.308197 -0.838620  
C -4.098625 1.834042 0.319138  
H -3.743366 2.486946 2.347774  
H -4.121345 1.139445 -1.729418  
H -5.160292 2.065328 0.333971  
H 3.349968 -0.284944 -1.678994  
CI -1.207078 -4.034721 0.918225  
CI -1.475149 0.399017 -2.363186  
H 2.984542 2.950117 2.165568  
H 3.395687 2.759804 -0.215170

\*\*\*\*

LOR TS2 1w

C -0.104687 0.903388 0.257306  
C -1.273844 1.563377 0.690904  
C 0.056755 -0.571348 0.338523  
C -2.996517 -0.243005 0.765291  
C -2.239467 -1.253828 0.076763  
O -4.261479 -0.268124 0.816179  
N -0.887745 -1.439497 0.238888  
N -2.361530 0.884189 1.301081  
C -1.364078 2.958113 0.576465  
C -0.320393 3.714724 0.047947  
H -0.402452 4.794328 -0.022781  
C 0.827686 3.058772 -0.392192  
C 0.935847 1.676104 -0.289534  
H 1.839596 1.183175 -0.630148  
H -2.264550 3.463248 0.918813  
O -2.920557 -2.531614 0.053023  
C 1.441370 -1.115207 0.526414  
C 2.168618 -0.749520 1.673451  
C 2.054194 -2.011441 -0.366150  
C 3.433545 -1.270501 1.938748  
H 1.714646 -0.050918 2.371808  
C 3.323303 -2.539311 -0.114771  
C 4.011582 -2.172894 1.041845  
H 3.962977 -0.975913 2.840659  
H 3.765769 -3.225184 -0.830197  
H 4.997732 -2.587028 1.233912  
H -3.080217 1.524556 1.627232  
H -3.180785 -0.912400 -1.272925  
CI 2.153909 3.986592 -1.078412  
CI 1.273123 -2.473131 -1.875522  
O -4.253702 -1.045795 -1.559695  
H -4.584001 -0.771274 -0.591652  
H -4.301848 -2.025358 -1.550425  
H -2.219069 -3.179194 0.240665

\*\*\*\*

LOR TS2 2w

C -0.266079 0.932345 -0.322982  
C 0.803774 1.691034 -0.841070  
C -0.295248 -0.551357 -0.413654  
C 2.656246 0.037025 -1.087973  
C 2.064955 -0.970081 -0.252374  
O 3.877433 0.060304 -1.417012  
N 0.734909 -1.321048 -0.352077  
N 1.868643 1.093413 -1.561799  
C 0.791158 3.087166 -0.713390  
C -0.263252 3.749198 -0.086800  
H -0.265555 4.831079 -0.004322  
C -1.312313 2.994946 0.435995  
C -1.317393 1.608683 0.320610  
H -2.147659 1.039323 0.723996  
H 1.614852 3.667337 -1.123829  
O 2.911557 -2.107937 -0.076839  
C -1.631072 -1.218304 -0.542050  
C -2.450955 -0.895334 -1.638959  
C -2.115581 -2.184192 0.357230  
C -3.678523 -1.519568 -1.851337  
H -2.098723 -0.144591 -2.342005  
C -3.345502 -2.817164 0.158685  
C -4.125969 -2.489014 -0.949872  
H -4.280209 -1.253022 -2.716020  
H -3.686304 -3.554693 0.878411  
H -5.081156 -2.984996 -1.100307  
H 2.463900 1.766327 -2.034796  
H 2.683976 -0.470466 1.282721  
CI -2.647867 3.804702 1.246002  
CI -1.221712 -2.607747 1.814731  
O 3.414070 -0.499766 2.056823  
H 4.803137 -0.494262 -0.345652  
H 2.646689 -2.785091 -0.724301  
O 5.322086 -0.616012 0.554332  
H 4.424021 -0.572628 1.388878  
H 3.278385 -1.372427 2.469957  
H 5.915985 0.148314 0.641161

\*\*\*\*

LOR TS4 0w

C 0.930800 -0.110368 0.072450  
C 2.111542 0.609297 0.414394  
C -0.409642 0.492420 0.145602  
C 1.442805 3.076615 0.437179  
C 0.369827 2.787548 -0.630240  
O 1.735881 4.166265 0.875716  
N -0.561344 1.758855 -0.037960  
N 2.135473 1.930553 0.879002  
C 3.342119 -0.078796 0.379123  
C 3.429535 -1.410359 0.001969  
H 4.392224 -1.910727 -0.023619  
C 2.266077 -2.100086 -0.358202  
C 1.037042 -1.463875 -0.313393  
H 0.139269 -2.009854 -0.581004  
H 4.248816 0.457900 0.646402

O -0.569450 3.713158 -0.889176  
C -1.596103 -0.336540 0.499820  
C -1.569317 -1.069119 1.700075  
C -2.761128 -0.390758 -0.287207  
C -2.671517 -1.809740 2.119327  
H -0.672403 -1.036916 2.312312  
C -3.865275 -1.142222 0.122337  
C -3.822187 -1.843982 1.326927  
H -2.631850 -2.356362 3.056832  
H -4.748220 -1.173871 -0.507584  
H -4.687467 -2.421419 1.640323  
H 2.953204 2.182079 1.427289  
Cl 2.367048 -3.777100 -0.859478  
H -1.325306 2.655843 -0.274777  
Cl -2.856359 0.432704 -1.831577  
H 0.892203 2.346619 -1.508819

\*\*\*\*

LOR TS4 1w

C -0.986904 -0.438765 0.068279  
C -1.452656 -1.722945 0.461192  
C 0.435717 -0.068039 0.122318  
C 0.649708 -3.137819 0.503522  
C 1.202429 -2.312928 -0.697061  
O 1.207856 -4.079678 1.021265  
N 1.376003 -0.913897 -0.126904  
N -0.615893 -2.729067 0.952381  
C -2.841012 -1.965442 0.456948  
C -3.747898 -0.993964 0.061489  
H -4.812131 -1.206354 0.057901  
C -3.279037 0.262220 -0.344202  
C -1.922820 0.540612 -0.328335  
H -1.570042 1.521348 -0.627584  
H -3.203948 -2.943181 0.763166  
O 2.350952 -2.751956 -1.210793  
C 0.816132 1.320014 0.521814  
C 0.414046 1.790563 1.784132  
C 1.589445 2.167309 -0.293073  
C 0.797229 3.049519 2.240010  
H -0.192700 1.146129 2.414652  
C 1.965571 3.436038 0.154797  
C 1.577717 3.871071 1.421922  
H 0.488313 3.386816 3.224970  
H 2.556509 4.073388 -0.494673  
H 1.880625 4.856769 1.764093  
H -1.044182 -3.407262 1.575570  
H 0.387151 -2.239904 -1.444059  
Cl -4.418800 1.488565 -0.862953  
H 3.276171 -2.107041 -0.698063  
Cl 2.050419 1.695620 -1.914614  
H 2.513907 -0.760627 0.021893  
O 3.827534 -1.195126 -0.133956  
H 4.265298 -1.521056 0.667804

\*\*\*\*

LOR TS4 2w

C -1.031138 -0.695620 0.039775  
C -1.042759 -2.043111 0.488433

C 0.194603 0.125101 0.053597  
C 1.397674 -2.679337 0.451818  
C 1.581616 -1.761190 -0.790041  
O 2.272356 -3.356634 0.952433  
N 1.356790 -0.361062 -0.226083  
N 0.097312 -2.700323 0.964686  
C -2.273233 -2.726215 0.547005  
C -3.457775 -2.121458 0.153380  
H -4.393874 -2.668700 0.196375  
C -3.434673 -0.801085 -0.313072  
C -2.244251 -0.094035 -0.355700  
H -2.239862 0.934900 -0.698206  
H -2.287399 -3.755176 0.896892  
O 2.740603 -1.876657 -1.423695  
C 0.090807 1.557484 0.465009  
C -0.464941 1.854698 1.722012  
C 0.546857 2.626717 -0.326684  
C -0.535817 3.163632 2.191504  
H -0.825868 1.037411 2.340305  
C 0.462737 3.943613 0.130010  
C -0.069582 4.209846 1.391429  
H -0.952862 3.365078 3.173743  
H 0.812216 4.749899 -0.506441  
H -0.124028 5.236449 1.742816  
H -0.052445 -3.447042 1.636774  
H 0.723808 -1.943721 -1.463625  
Cl -4.924590 -0.037569 -0.832153  
H 3.737951 -1.710957 -0.724091  
Cl 1.184424 2.360428 -1.940798  
H 2.349084 0.243804 0.007445  
O 4.657972 -1.340471 -0.048824  
H 4.739928 -1.950808 0.700375  
O 3.523010 0.736133 0.449099  
H 3.866011 1.419725 -0.147848  
H 4.179189 -0.222968 0.292486

\*\*\*\*

XYZ coordinates for Table S8

LMZ 1ax 0w

C 0.447582 0.341327 -0.267599  
 C -0.303354 -0.915790 -0.546052  
 C 1.753892 0.338073 0.285027  
 C 2.465003 -2.007883 -0.117209  
 C -0.169181 1.570622 -0.563643  
 H -1.171473 1.574496 -0.978526  
 C 0.483444 2.772239 -0.325978  
 C 1.765629 2.781206 0.226800  
 C 2.385909 1.573235 0.524597  
 H 3.387608 1.588264 0.939827  
 H 2.276897 3.720233 0.412122  
 N 2.422374 -0.851118 0.655434  
 C -1.784074 -0.925912 -0.312261  
 C -2.389199 -0.601911 0.913191  
 C -2.622449 -1.308118 -1.373409  
 C -3.775446 -0.635572 1.072237  
 C -4.008523 -1.336494 -1.230969  
 H -2.158736 -1.583556 -2.315625  
 C -4.585931 -0.994464 -0.005687  
 H -4.208340 -0.392666 2.037313  
 H -4.633207 -1.627461 -2.070686  
 H -5.665073 -1.014459 0.119969  
 O 3.145026 -2.968246 0.208977  
 Cl -0.307439 4.287989 -0.719538  
 C 1.611552 -2.040614 -1.401383  
 N 0.198689 -1.987391 -1.043642  
 O 2.032339 -1.114528 -2.392763  
 H 1.862936 -0.203792 -2.102500  
 H 1.801644 -3.015397 -1.846983  
 C 3.304971 -0.831720 1.831639  
 H 3.335766 -1.838494 2.248249  
 H 4.328977 -0.541125 1.567028  
 H 2.900780 -0.135952 2.568994  
 Cl -1.416272 -0.209617 2.328525

\*\*\*\*

LMZ 1eq 0w

C 0.648618 -0.452598 -0.049556  
 C 2.003316 -0.212440 0.289015  
 C -0.379717 0.626782 -0.027882  
 C 2.119290 2.244079 0.126685  
 C 1.108083 2.156296 -1.029374  
 O 2.558167 3.328149 0.491533  
 N -0.181624 1.824233 -0.440015  
 N 2.458584 1.055504 0.736390  
 C 2.914757 -1.282966 0.255906  
 C 2.515580 -2.563279 -0.110058  
 H 3.234879 -3.375230 -0.140727  
 C 1.178966 -2.791232 -0.446518  
 C 0.255954 -1.755096 -0.408181  
 H -0.782470 -1.946436 -0.657245  
 H 3.955060 -1.108866 0.509728  
 O 1.067779 3.365186 -1.717769  
 C -1.727732 0.289447 0.534078  
 C -1.806276 -0.215206 1.843383

C -2.931227 0.483539 -0.166009  
 C -3.030653 -0.485424 2.451242  
 H -0.883218 -0.382118 2.392772  
 C -4.164240 0.205447 0.430592  
 C -4.214193 -0.270750 1.740587  
 H -3.060078 -0.860814 3.470220  
 H -5.075334 0.359919 -0.138484  
 H -5.177241 -0.479594 2.198517  
 H 1.415977 1.384016 -1.748643  
 Cl 0.663825 -4.401567 -0.915459  
 H 1.332975 4.063929 -1.089166  
 C 3.461656 1.123362 1.809410  
 H 4.482758 1.079524 1.412111  
 H 3.339018 2.074039 2.328965  
 H 3.301103 0.295613 2.502871  
 Cl -2.942813 1.024591 -1.835457

\*\*\*\*

LMZ 1eq 1w

C -0.973566 0.200880 -0.024000  
 C -2.041366 -0.680565 0.278273  
 C 0.451125 -0.224066 0.024240  
 C -0.941873 -2.880731 0.117641  
 C -0.053665 -2.299504 -0.996022  
 O -0.822438 -4.051897 0.455711  
 N 0.879106 -1.365695 -0.375057  
 N -1.827517 -2.014099 0.716461  
 C -3.360223 -0.195774 0.221869  
 C -3.634364 1.120339 -0.131223  
 H -4.659369 1.473059 -0.179955  
 C -2.576397 1.982813 -0.429535  
 C -1.264527 1.534348 -0.367246  
 H -0.449127 2.215037 -0.586640  
 H -4.185697 -0.862261 0.447966  
 O 0.624655 -3.330486 -1.641206  
 C 1.450958 0.740419 0.587235  
 C 1.342520 1.120860 1.934843  
 C 2.517515 1.262538 -0.162330  
 C 2.281226 1.961770 2.529199  
 H 0.515138 0.731505 2.522861  
 C 3.458787 2.113639 0.421294  
 C 3.344087 2.455592 1.768512  
 H 2.184907 2.227555 3.577968  
 H 4.272156 2.501506 -0.183132  
 H 4.083987 3.111651 2.218742  
 H -0.667845 -1.779792 -1.745321  
 Cl -2.910263 3.644149 -0.879268  
 H 0.625732 -4.096021 -1.032012  
 C -2.699475 -2.578146 1.758881  
 H -3.594461 -3.043549 1.329434  
 H -2.138811 -3.346186 2.292381  
 H -2.991579 -1.783520 2.447728  
 Cl 2.676854 0.916084 -1.876569  
 O 3.615210 -2.596536 -0.143003  
 H 3.722445 -3.035745 -0.999735  
 H 2.745345 -2.153767 -0.212684

\*\*\*\*

LMZ 1eq 2w

C -0.573098 0.841589 0.134674  
 C -1.880141 0.703587 0.665434  
 C 0.426864 -0.259305 0.175402  
 C -2.089768 -1.740596 0.864406  
 C -1.214363 -1.856698 -0.393304  
 O -2.523831 -2.748235 1.409383  
 N 0.144674 -1.495624 -0.026667  
 N -2.308647 -0.470328 1.340483  
 C -2.763006 1.795111 0.592307  
 C -2.383004 2.996562 0.005981  
 H -3.082811 3.823774 -0.052747  
 C -1.093637 3.124796 -0.516627  
 C -0.197490 2.067566 -0.445588  
 H 0.805413 2.181294 -0.842769  
 H -3.768144 1.697809 0.988316  
 O -1.267771 -3.175724 -0.866821  
 C 1.848051 0.095347 0.484418  
 C 2.132165 0.757100 1.691057  
 C 2.925912 -0.229310 -0.356960  
 C 3.439870 1.053954 2.068330  
 H 1.307002 1.023326 2.346636  
 C 4.239754 0.073057 0.007352  
 C 4.496436 0.706639 1.222967  
 H 3.632218 1.550974 3.014758  
 H 5.050818 -0.188182 -0.664372  
 H 5.521823 0.931782 1.503040  
 H -1.592819 -1.204717 -1.192074  
 Cl -0.604210 4.634164 -1.262036  
 H -1.560225 -3.734658 -0.116717  
 C -3.178183 -0.348953 2.521470  
 H -4.237672 -0.328551 2.241205  
 H -3.009691 -1.218153 3.157788  
 H -2.920910 0.563808 3.061798  
 Cl 2.669094 -0.969054 -1.929673  
 O 1.919854 -3.814689 0.652801  
 H 2.095114 -4.292950 -0.170817  
 H 1.353131 -3.062584 0.385031  
 O -3.015903 -2.620228 -3.027760  
 H -2.840301 -3.040745 -3.881608  
 H -2.425129 -3.059104 -2.383845

\*\*\*\*

LMZ An1 0w

C -0.647946 0.468856 0.110499  
 C -2.004567 0.088659 0.293380  
 C 0.437196 -0.510035 0.156532  
 C -2.073316 -2.329425 0.130415  
 C -0.776285 -2.464346 -0.500607  
 O -2.897207 -3.274248 0.116263  
 N 0.300872 -1.767591 -0.283386  
 N -2.300664 -1.179302 0.908433  
 C -3.040475 0.980129 -0.004766  
 C -2.787052 2.299219 -0.396654  
 H -3.595903 2.998525 -0.580657  
 C -1.452035 2.688175 -0.517268  
 C -0.405080 1.809350 -0.291051  
 H 0.616793 2.140448 -0.439344  
 H -4.070911 0.661521 0.122983

O -0.625400 -3.669074 -1.180811  
C 1.803638 -0.069340 0.495970  
C 1.986592 0.776778 1.621558  
C 2.999175 -0.442515 -0.171227  
C 3.234351 1.200651 2.064109  
H 1.096348 1.078670 2.167360  
C 4.260146 -0.041248 0.277025  
C 4.392454 0.780117 1.398062  
H 3.305312 1.842315 2.940335  
H 5.137573 -0.361698 -0.277757  
H 5.379173 1.088026 1.736023  
Cl -1.087945 4.360875 -1.004184  
H -1.465047 -4.142433 -1.015204  
C -3.448725 -1.249222 1.803043  
H -4.417569 -1.275758 1.279953  
H -3.377090 -2.163609 2.397278  
H -3.422330 -0.378855 2.466205  
Cl 2.977628 -1.374237 -1.670537

\*\*\*\*

LMZ An1 1w

C -0.088691 0.730422 0.114414  
C -1.487334 0.850676 0.313051  
C 0.581920 -0.572641 0.159902  
C -2.396665 -1.375039 0.129458  
C -1.245533 -1.964152 -0.496048  
O -3.516542 -1.965134 0.091545  
N 0.015592 -1.698752 -0.272052  
N -2.198236 -0.238494 0.929338  
C -2.149034 2.048237 0.021542  
C -1.449450 3.190683 -0.380121  
H -1.961452 4.130586 -0.558309  
C -0.064871 3.085374 -0.520371  
C 0.608546 1.893739 -0.299902  
H 1.679965 1.842579 -0.459520  
H -3.224173 2.110798 0.161481  
O -1.523493 -3.134489 -1.195917  
C 2.019685 -0.635835 0.499862  
C 2.479689 0.077717 1.635779  
C 3.009703 -1.386481 -0.182077  
C 3.797762 0.038288 2.077399  
H 1.747774 0.660310 2.189293  
C 4.332820 -1.449720 0.262762  
C 4.738685 -0.742611 1.395699  
H 4.086837 0.601423 2.962498  
H 5.046448 -2.042755 -0.302088  
H 5.771520 -0.797714 1.731497  
Cl 0.858076 4.520711 -1.019529  
H -2.472414 -3.296652 -1.028080  
C -3.264488 0.086948 1.871186  
H -4.192167 0.436020 1.395414  
H -3.507952 -0.808055 2.449838  
H -2.894986 0.863644 2.548260  
Cl 2.661592 -2.232406 -1.690445  
O -6.162509 -1.109680 0.043172  
H -6.326276 -1.221502 -0.904211  
H -5.225078 -1.398349 0.156851

\*\*\*\*

LMZ An1 2w

C 0.234440 0.698669 0.064081  
C -1.173251 0.742985 0.213879  
C 0.976540 -0.565376 0.156455  
C -1.942152 -1.532326 0.014929  
C -0.740574 -2.063976 -0.551688  
O -3.029669 -2.186402 -0.066891  
N 0.496614 -1.726563 -0.276909  
N -1.842096 -0.381602 0.812988  
C -1.890025 1.899742 -0.111854  
C -1.238546 3.072670 -0.505683  
H -1.794795 3.981315 -0.710891  
C 0.152943 3.041760 -0.602959  
C 0.882187 1.890547 -0.345045  
H 1.959530 1.895096 -0.468761  
H -2.970791 1.907813 -0.006004  
O -0.918929 -3.254107 -1.251485  
C 2.401410 -0.538141 0.556728  
C 2.767570 0.204107 1.707332  
C 3.462028 -1.225957 -0.082450  
C 4.066727 0.248168 2.202070  
H 1.978676 0.740510 2.228340  
C 4.767862 -1.204059 0.414614  
C 5.081469 -0.471392 1.560454  
H 4.284021 0.829339 3.095890  
H 5.539996 -1.750860 -0.118984  
H 6.101526 -0.459798 1.937104  
Cl 1.012880 4.518252 -1.091514  
H -1.861292 -3.474259 -1.118293  
C -2.953577 -0.110061 1.718694  
H -3.877183 0.212468 1.217614  
H -3.177365 -1.019899 2.282214  
H -2.640756 0.675055 2.414466  
Cl 3.225937 -2.096566 -1.597857  
O -5.656564 -1.640075 -0.332169  
H -5.749344 -1.736531 -1.290907  
H -4.688769 -1.798072 -0.155511  
O -6.810299 0.681432 0.695852  
H -7.170803 0.370433 1.538525  
H -6.380795 -0.115058 0.302128

\*\*\*\*

LMZ An2 0w

C 0.633469 -0.429548 -0.053755  
C 1.998995 -0.232513 0.287111  
C -0.346304 0.698645 -0.067423  
C 2.202245 2.263209 0.079524  
C 1.252063 2.199499 -1.183404  
O 2.737382 3.270393 0.506333  
N -0.114064 1.880941 -0.490204  
N 2.496623 1.011363 0.709774  
C 2.856184 -1.355265 0.287604  
C 2.402773 -2.629035 -0.039767  
H 3.085955 -3.473042 -0.044502  
C 1.059017 -2.802655 -0.369186  
C 0.185388 -1.723826 -0.367572  
H -0.861236 -1.874267 -0.612876  
H 3.904961 -1.223546 0.532127

O 1.239801 3.236524 -1.939519  
C -1.703859 0.420151 0.524989  
C -1.796829 0.077178 1.886150  
C -2.910087 0.538775 -0.185765  
C -3.023744 -0.106765 2.522102  
H -0.873163 -0.029698 2.450106  
C -4.148638 0.352540 0.435297  
C -4.208091 0.036045 1.793309  
H -3.055302 -0.357905 3.579814  
H -5.056811 0.452303 -0.151682  
H -5.174317 -0.102614 2.272839  
Cl 0.464792 -4.418512 -0.786165  
C 3.565822 1.029170 1.706995  
H 4.562875 0.905400 1.257627  
H 3.543334 2.002837 2.198327  
H 3.402629 0.233168 2.440415  
H 1.528512 1.229003 -1.691259  
Cl -2.912630 0.884586 -1.910287

\*\*\*\*

LMZ An2 1w

C 0.751386 0.513057 0.000696  
C 2.094835 0.186790 -0.323091  
C -0.372524 -0.431108 -0.266094  
C 1.938085 -2.295358 -0.658446  
C 0.909143 -2.349741 0.526551  
O 2.355950 -3.263187 -1.266210  
N -0.334690 -1.697025 -0.100044  
N 2.439679 -1.002167 -0.990165  
C 3.100287 1.138136 -0.045373  
C 2.808080 2.370066 0.530265  
H 3.600968 3.080279 0.744275  
C 1.481808 2.675467 0.835929  
C 0.467501 1.766646 0.569529  
H -0.561514 2.020254 0.803158  
H 4.134469 0.900340 -0.271085  
O 0.698938 -3.539457 1.010468  
C -1.639467 0.162703 -0.825952  
C -1.609319 0.749840 -2.102966  
C -2.879095 0.123443 -0.167398  
C -2.759377 1.247650 -2.714040  
H -0.655507 0.796567 -2.623207  
C -4.040737 0.622739 -0.764038  
C -3.983184 1.179817 -2.042061  
H -2.701355 1.682450 -3.709010  
H -4.979482 0.574894 -0.220532  
H -4.890258 1.562205 -2.504143  
Cl 1.093258 4.240002 1.564728  
C 3.551248 -0.969117 -1.940845  
H 4.526397 -1.106797 -1.450718  
H 3.414124 -1.793266 -2.642076  
H 3.549823 -0.014944 -2.476209  
H 1.284403 -1.596517 1.272363  
Cl -3.011532 -0.515326 1.465204  
O -1.224322 -3.660371 2.876348  
H -1.951578 -3.324269 2.331628  
H -0.451321 -3.648388 2.227343

\*\*\*\*

LMZ An2 2w

C 0.551258 0.870186 0.060094  
 C -0.188594 2.012046 0.461801  
 C 0.018929 -0.512315 0.236603  
 C -2.479098 1.046669 0.729769  
 C -2.188588 0.133669 -0.508351  
 O -3.536229 1.080780 1.338623  
 N -1.192417 -0.869032 0.042334  
 N -1.429024 1.910601 1.121936  
 C 0.385271 3.286431 0.271650  
 C 1.644743 3.445712 -0.295875  
 H 2.061170 4.437386 -0.443105  
 C 2.360742 2.312242 -0.682218  
 C 1.827860 1.043850 -0.502408  
 H 2.398385 0.169454 -0.798132  
 H -0.174041 4.170306 0.559798  
 O -3.254310 -0.417465 -1.050960  
 C 0.987195 -1.554907 0.729177  
 C 1.575566 -1.391037 1.995128  
 C 1.312239 -2.719610 0.014979  
 C 2.423902 -2.351028 2.544783  
 H 1.341552 -0.490113 2.557278  
 C 2.166291 -3.688761 0.550213  
 C 2.717929 -3.508466 1.818796  
 H 2.849645 -2.197926 3.533395  
 H 2.394368 -4.575158 -0.033682  
 H 3.377007 -4.268232 2.231942  
 Cl 3.963672 2.498731 -1.402505  
 C -1.750461 2.891061 2.161263  
 H -2.209998 3.800140 1.748006  
 H -2.470436 2.434396 2.841423  
 H -0.840035 3.160877 2.703677  
 H -1.617788 0.776851 -1.222875  
 Cl 0.696905 -2.988376 -1.608626  
 O -2.959167 -0.691486 -3.697289  
 H -2.644040 -1.606493 -3.727387  
 H -3.131496 -0.544905 -2.714976  
 O -5.327316 -1.282770 0.561955  
 H -4.599395 -1.105182 -0.092068  
 H -5.189570 -0.535321 1.164978

\*\*\*\*

LMZ Cat1 0w

C 0.688174 -0.456978 -0.027968  
 C 2.034824 -0.114977 0.267239  
 C -0.435582 0.514768 0.013941  
 C 2.004343 2.322461 0.160843  
 C 0.913363 2.185550 -0.919879  
 O 2.352209 3.471987 0.456084  
 N -0.318131 1.741949 -0.373184  
 N 2.429289 1.183237 0.733508  
 C 3.027741 -1.100917 0.177803  
 C 2.722200 -2.401311 -0.209637  
 H 3.506648 -3.147184 -0.284998  
 C 1.398441 -2.738029 -0.507741  
 C 0.394811 -1.780865 -0.407752  
 H -0.629873 -2.053218 -0.634618  
 H 4.058085 -0.850846 0.406407

O 0.697224 3.518890 -1.307582  
 C -1.759588 0.068514 0.516517  
 C -1.808791 -0.634718 1.736392  
 C -2.978231 0.348751 -0.136776  
 C -3.020206 -1.014344 2.307077  
 H -0.878949 -0.864001 2.249386  
 C -4.193608 -0.048699 0.421574  
 C -4.214765 -0.719038 1.645813  
 H -3.031454 -1.540371 3.256626  
 H -5.116252 0.162606 -0.108709  
 H -5.167346 -1.017212 2.073944  
 H 1.250273 1.635132 -1.806104  
 Cl 1.002580 -4.358851 -1.001439  
 H -0.228844 3.741163 -1.186782  
 H 1.238799 4.100532 -0.769076  
 C 3.450763 1.301644 1.798666  
 H 4.459707 1.306303 1.375401  
 H 3.287825 2.241729 2.325867  
 H 3.336289 0.463370 2.486253  
 Cl -3.037980 1.125192 -1.710946

\*\*\*\*

LMZ Cat1 1w

C 1.036042 -0.052405 -0.042684  
 C 1.902401 1.020883 0.287495  
 C -0.443531 0.023047 0.091670  
 C 0.361673 2.909667 0.388894  
 C -0.448747 2.211140 -0.724732  
 O -0.058853 3.995004 0.796682  
 N -1.132863 1.071725 -0.210281  
 N 1.431564 2.241693 0.866275  
 C 3.285791 0.863689 0.117168  
 C 3.820705 -0.317512 -0.385278  
 H 4.892487 -0.417362 -0.521840  
 C 2.966551 -1.373086 -0.719629  
 C 1.593917 -1.245744 -0.539719  
 H 0.941287 -2.074239 -0.791956  
 H 3.955821 1.677470 0.372795  
 O -1.398901 3.183669 -1.080009  
 C -1.166827 -1.167634 0.618491  
 C -0.667515 -1.781781 1.783634  
 C -2.348253 -1.694373 0.061986  
 C -1.327511 -2.849316 2.386725  
 H 0.245427 -1.396649 2.228677  
 C -3.006108 -2.775817 0.646257  
 C -2.500336 -3.346868 1.815593  
 H -0.925736 -3.291926 3.292942  
 H -3.903291 -3.170681 0.181236  
 H -3.021191 -4.185109 2.268881  
 H 0.156641 2.004997 -1.615671  
 Cl 3.622528 -2.854841 -1.357235  
 H -2.272326 2.785724 -1.099191  
 H -1.385354 3.894824 -0.435281  
 C 2.207743 2.889955 1.945873  
 H 2.968789 3.560401 1.534656  
 H 1.520846 3.474765 2.557834  
 H 2.679630 2.115378 2.551014  
 Cl -3.018120 -1.086964 -1.454946  
 O -3.746788 2.228192 -1.090287

H -4.449498 2.443586 -1.724484  
 H -3.729001 1.257586 -0.986043

\*\*\*\*

LMZ Cat1 2w

C -1.318418 0.306291 0.082285  
 C -1.755819 1.619562 -0.226179  
 C 0.040905 -0.197098 -0.252042  
 C 0.349424 2.769182 -0.681183  
 C 0.998984 1.840774 0.366973  
 O 1.072718 3.606438 -1.224689  
 N 1.111537 0.513097 -0.139344  
 N -0.952684 2.546754 -0.961457  
 C -3.053865 2.012168 0.133166  
 C -3.911023 1.144312 0.800815  
 H -4.907329 1.469209 1.082022  
 C -3.476697 -0.147485 1.113566  
 C -2.201724 -0.564012 0.748894  
 H -1.878227 -1.571738 0.985325  
 H -3.399184 3.012887 -0.103457  
 O 2.287801 2.379193 0.521655  
 C 0.173300 -1.592120 -0.759095  
 C -0.682635 -2.004378 -1.798569  
 C 1.132773 -2.515256 -0.300237  
 C -0.570778 -3.264867 -2.379732  
 H -1.434353 -1.310707 -2.164459  
 C 1.239415 -3.787137 -0.862325  
 C 0.393975 -4.157983 -1.909284  
 H -1.234957 -3.548411 -3.190349  
 H 1.976243 -4.482312 -0.473828  
 H 0.487331 -5.147934 -2.346106  
 H 0.499510 1.902644 1.341577  
 Cl -4.538048 -1.242120 1.956865  
 H 2.938609 1.677177 0.449532  
 H 2.445525 3.033358 -0.163037  
 C -1.580656 3.417266 -1.978460  
 H -1.952112 4.343663 -1.529236  
 H -0.827355 3.669888 -2.724856  
 H -2.401618 2.873566 -2.446821  
 Cl 2.193041 -2.158678 1.063239  
 O 4.082026 0.673787 0.292993  
 H 4.913841 0.673689 0.824424  
 H 3.742760 -0.237256 0.256181  
 O 6.452951 0.756978 1.677345  
 H 7.305933 0.773118 1.215732  
 H 6.651609 0.657283 2.621211

\*\*\*\*

LMZ Cat2 0w

C 0.677836 -0.459415 -0.035420  
 C 2.025640 -0.141113 0.258242  
 C -0.432851 0.535817 -0.001345  
 C 1.965774 2.254532 0.131804  
 C 0.937652 2.188037 -0.984190  
 O 2.335505 3.427719 0.553552  
 N -0.306808 1.754065 -0.404269  
 N 2.423433 1.171133 0.712015  
 C 3.018750 -1.124672 0.183350

C 2.702341 -2.423576 -0.199685  
H 3.479528 -3.176954 -0.273314  
C 1.374026 -2.748264 -0.494833  
C 0.374997 -1.782745 -0.401438  
H -0.652038 -2.049089 -0.624953  
H 4.050680 -0.878136 0.410759  
O 0.810763 3.510995 -1.460760  
C -1.757017 0.101448 0.517880  
C -1.806216 -0.566906 1.756696  
C -2.974569 0.364167 -0.143746  
C -3.017615 -0.928298 2.339441  
H -0.876690 -0.785075 2.275882  
C -4.190399 -0.014330 0.428328  
C -4.212242 -0.648803 1.671125  
H -3.029171 -1.427171 3.303594  
H -5.112979 0.184824 -0.106786  
H -5.165036 -0.931941 2.108904  
H 1.295247 1.527382 -1.788604  
Cl 0.965898 -4.366322 -0.977966  
H 1.881842 4.086097 -0.039439  
H -0.141516 3.725719 -1.474024  
C 3.394488 1.292900 1.832184  
H 4.412928 1.361787 1.440625  
H 3.166303 2.193160 2.402396  
H 3.292098 0.414729 2.467915  
Cl -3.028915 1.094315 -1.736733

\*\*\*\*

LMZ Cat2 1w

C 0.375654 0.893069 -0.022817  
C -0.594724 1.875568 0.283908  
C 0.092885 -0.568179 0.024999  
C -2.634174 0.579881 0.231573  
C -2.051503 -0.231734 -0.916926  
O -3.797258 0.337167 0.729489  
N -1.027893 -1.079552 -0.352549  
N -1.902410 1.532621 0.784129  
C -0.277157 3.235750 0.180874  
C 0.985968 3.640379 -0.236493  
H 1.219670 4.695647 -0.330614  
C 1.951786 2.674275 -0.538955  
C 1.654418 1.319698 -0.422938  
H 2.412237 0.579679 -0.655488  
H -1.023461 3.988074 0.415003  
O -3.060428 -1.026802 -1.480236  
C 1.153913 -1.483274 0.526890  
C 1.779467 -1.178494 1.750949  
C 1.539647 -2.664863 -0.138696  
C 2.725399 -2.029548 2.315952  
H 1.500299 -0.266611 2.272180  
C 2.500326 -3.512676 0.415888  
C 3.083843 -3.201000 1.644495  
H 3.181168 -1.778946 3.268940  
H 2.790600 -4.409001 -0.122137  
H 3.825614 -3.871627 2.068486  
H -1.660798 0.461604 -1.678439  
Cl 3.534748 3.168676 -1.063043  
H -4.360718 -0.368203 0.244932  
H -2.767699 -1.951865 -1.376924

C -2.456686 2.290547 1.935779  
H -3.153106 3.057658 1.586044  
H -2.986541 1.600205 2.592444  
H -1.628476 2.749162 2.472963  
Cl 0.906776 -3.092250 -1.717247  
O -5.549476 -1.327622 -0.208316  
H -5.602757 -1.416227 -1.173858  
H -6.456878 -1.238609 0.125955

\*\*\*\*

LMZ Cat2 2w

C -1.044340 -0.659853 -0.047328  
C -0.763121 -2.017203 0.239420  
C -0.018881 0.419258 0.042380  
C 1.649951 -1.991981 0.251085  
C 1.599909 -1.006552 -0.910861  
O 2.752763 -2.373265 0.790727  
N 1.204911 0.261075 -0.328921  
N 0.511112 -2.436246 0.762216  
C -1.762306 -2.988308 0.097813  
C -3.035837 -2.639387 -0.337719  
H -3.800221 -3.399359 -0.461168  
C -3.321197 -1.299378 -0.621072  
C -2.342828 -0.321839 -0.468046  
H -2.578059 0.713869 -0.687274  
H -1.543205 -4.028583 0.316136  
O 2.848247 -0.925025 -1.514749  
C -0.432377 1.742265 0.589206  
C -1.146099 1.772254 1.802602  
C -0.116726 2.973520 -0.019698  
C -1.505117 2.973437 2.408468  
H -1.406467 0.832484 2.282214  
C -0.491191 4.181020 0.572974  
C -1.175222 4.181259 1.789342  
H -2.042773 2.966359 3.351687  
H -0.252129 5.114084 0.073404  
H -1.457240 5.126728 2.243545  
H 0.867464 -1.378856 -1.644573  
Cl -4.911002 -0.850939 -1.169220  
H 3.620854 -1.929365 0.447301  
H 3.229154 -0.032051 -1.371242  
C 0.548511 -3.383518 1.904986  
H 0.716993 -4.403205 1.547439  
H 1.363345 -3.101024 2.571697  
H -0.401582 -3.322247 2.433321  
Cl 0.687191 3.061585 -1.578278  
O 5.067574 -1.318033 0.493886  
H 5.163348 -0.499393 -0.038139  
H 5.811779 -1.899462 0.271926  
O 4.704637 1.107940 -0.938896  
H 5.225200 1.474262 -1.672988  
H 4.431639 1.868080 -0.397950

\*\*\*\*

LMZ Cat3 0w

C -0.700277 0.436775 -0.038968  
C -2.028901 0.026833 0.286385  
C 0.462881 -0.448676 0.024703

C -1.940444 -2.428490 0.195209  
C -0.894339 -2.301559 -0.932023  
O -2.310098 -3.542131 0.530935  
N 0.320447 -1.705388 -0.323724  
N -2.354609 -1.262221 0.784203  
C -3.057168 0.979392 0.199602  
C -2.813940 2.283221 -0.214980  
H -3.633148 2.991110 -0.290668  
C -1.512189 2.678452 -0.548226  
C -0.469260 1.770079 -0.451115  
H 0.534948 2.079417 -0.716781  
H -4.072411 0.690410 0.447209  
O -0.564973 -3.538723 -1.429417  
C 1.772813 0.044869 0.481512  
C 1.791180 0.898053 1.608948  
C 3.013642 -0.309931 -0.104610  
C 2.986341 1.359162 2.147837  
H 0.850624 1.172853 2.075620  
C 4.209590 0.172905 0.423244  
C 4.196807 0.996730 1.550841  
H 2.973802 1.998542 3.024735  
H 5.146031 -0.093951 -0.055183  
H 5.137435 1.358229 1.955868  
H -1.229924 -1.626361 -1.729922  
Cl -1.203432 4.303913 -1.081882  
H -1.051756 -4.207447 -0.897792  
H 1.104961 -2.354154 -0.259392  
C -3.378539 -1.394639 1.845069  
H -4.382930 -1.484404 1.419315  
H -3.162592 -2.300792 2.411357  
H -3.322998 -0.524633 2.499953  
Cl 3.116283 -1.295547 -1.551082

\*\*\*\*

LMZ Cat3 1w

C -0.991699 0.233304 -0.022994  
C -2.073264 -0.653991 0.261793  
C 0.417870 -0.154028 0.043020  
C -1.048797 -2.885048 0.124520  
C -0.116442 -2.334183 -0.972789  
O -0.963167 -4.063375 0.436311  
N 0.783382 -1.356412 -0.318139  
N -1.895902 -1.986549 0.718184  
C -3.383052 -0.153586 0.180911  
C -3.641442 1.162070 -0.183982  
H -4.665206 1.515008 -0.255798  
C -2.578885 2.029170 -0.467551  
C -1.272910 1.573098 -0.377107  
H -0.453643 2.247024 -0.599315  
H -4.218715 -0.810344 0.394961  
O 0.634825 -3.347574 -1.520179  
C 1.438614 0.802523 0.519231  
C 1.217087 1.447189 1.753865  
C 2.626265 1.094813 -0.186551  
C 2.160793 2.317346 2.289538  
H 0.302651 1.237748 2.301214  
C 3.560454 1.986779 0.337423  
C 3.333564 2.585614 1.578196  
H 1.979525 2.788245 3.250536



H 4.455540 2.215295 -0.231446  
H 4.072374 3.272679 1.980266  
H -0.676414 -1.797935 -1.749692  
Cl -2.896639 3.675228 -0.931375  
H 0.438958 -4.161596 -1.006185  
H 1.760877 -1.686527 -0.173526  
C -2.809673 -2.529559 1.747464  
H -3.698255 -2.979422 1.293198  
H -2.275982 -3.304048 2.298559  
H -3.099428 -1.724493 2.423359  
Cl 2.932762 0.438179 -1.784753  
O 3.406684 -2.233484 0.258297  
H 4.012445 -2.292966 -0.498447  
H 3.581205 -3.019453 0.800813

\*\*\*\*

LMZ Cat3 2w

C 1.223314 0.313492 -0.019553  
C 1.543298 1.676829 0.253129  
C -0.147241 -0.198076 -0.099060  
C -0.560837 2.867527 -0.196294  
C -0.850897 1.828617 -1.297181  
O -1.354345 3.779863 -0.016301  
N -1.094321 0.539692 -0.612314  
N 0.569313 2.666340 0.551758  
C 2.897753 2.041406 0.325779  
C 3.914841 1.116875 0.121709  
H 4.952618 1.431263 0.165784  
C 3.597499 -0.219540 -0.149991  
C 2.270425 -0.616754 -0.208525  
H 2.029195 -1.652171 -0.420035  
H 3.161940 3.072418 0.532550  
O -1.967005 2.186750 -2.017309  
C -0.473911 -1.549526 0.403843  
C -0.079576 -1.883097 1.715661  
C -1.170341 -2.515172 -0.354864  
C -0.404975 -3.115657 2.272111  
H 0.466815 -1.151199 2.303504  
C -1.474988 -3.760062 0.193982  
C -1.104860 -4.053400 1.507671  
H -0.108477 -3.345853 3.290596  
H -1.992727 -4.495862 -0.412261  
H -1.354709 -5.023834 1.926597  
H 0.011629 1.693081 -1.962046  
Cl 4.866753 -1.380876 -0.412264  
H -2.360309 2.966757 -1.569185  
H -2.104367 0.245185 -0.552992  
C 0.859926 3.680481 1.587957  
H 1.372589 4.549183 1.162506  
H -0.088334 4.013332 2.010192  
H 1.474452 3.225696 2.365557  
Cl -1.590261 -2.238271 -2.033841  
O -3.711799 -0.200452 -0.248486  
H -4.239768 -0.376384 -1.042500  
H -4.272852 0.348549 0.346954  
O -5.199678 1.329559 1.529572  
H -5.545033 2.223826 1.380578  
H -5.801918 0.909885 2.163838

\*\*\*\*

LMZ TS2 0w

C 0.407504 0.434505 -0.176002  
C 1.732796 0.732761 0.207671  
C -0.163226 -0.932124 -0.394452  
C 2.754136 -1.424468 -0.029206  
C 1.842737 -2.084804 -0.999803  
O 3.662110 -2.300554 0.290662  
N 0.456709 -1.943361 -0.906464  
N 2.636532 -0.290569 0.649938  
C 2.190812 2.054263 0.233963  
C 1.357190 3.116031 -0.105339  
H 1.719863 4.137946 -0.081058  
C 0.044967 2.831388 -0.478572  
C -0.421456 1.523078 -0.515713  
H -1.444856 1.335612 -0.818686  
H 3.216259 2.258789 0.524881  
O 2.319526 -2.021421 -2.340883  
C -1.647191 -1.100463 -0.245748  
C -2.393076 -1.576389 -1.338498  
C -2.341503 -0.852644 0.948628  
C -3.770317 -1.767449 -1.253672  
H -1.859999 -1.795852 -2.258608  
C -3.721078 -1.043525 1.052223  
C -4.437988 -1.495691 -0.055545  
H -4.320944 -2.127189 -2.118567  
H -4.218953 -0.847812 1.996562  
H -5.511981 -1.641193 0.023548  
Cl -1.036261 4.144833 -0.913698  
H 2.427011 -2.922650 -2.677748  
H 2.912232 -3.036256 -0.304059  
C 3.457729 -0.059838 1.850700  
H 2.884472 0.543305 2.558693  
H 3.702538 -1.029762 2.286454  
H 4.391722 0.453143 1.599964  
Cl -1.478760 -0.335572 2.399714

\*\*\*\*

LMZ TS2 1w

C -0.204269 0.792713 0.159622  
C -1.528399 1.064163 0.568417  
C 0.388502 -0.562982 0.261033  
C -2.629635 -1.120685 0.538587  
C -1.600505 -1.805267 -0.205235  
O -3.829371 -1.520272 0.514038  
N -0.261608 -1.655788 0.055308  
N -2.323878 0.070796 1.227908  
C -2.051605 2.352224 0.368903  
C -1.286796 3.369925 -0.200028  
H -1.705145 4.362359 -0.332962  
C 0.020509 3.093835 -0.593745  
C 0.556960 1.823497 -0.419096  
H 1.576785 1.621886 -0.728521  
H -3.067364 2.577714 0.671620  
O -1.914737 -3.204241 -0.413823  
C 1.849101 -0.679022 0.562701  
C 2.351028 -0.046988 1.715858  
C 2.763366 -1.412158 -0.215837

C 3.686241 -0.158872 2.097195  
H 1.662228 0.530889 2.326667  
C 4.105750 -1.530485 0.153902  
C 4.567496 -0.908713 1.313972  
H 4.035268 0.333664 3.000609  
H 4.781349 -2.100529 -0.475875  
H 5.612384 -1.005838 1.596172  
H -2.551565 -1.558171 -1.571678  
Cl 1.002108 4.362243 -1.314620  
O -3.536595 -1.942683 -1.938600  
H -3.955321 -1.903622 -0.968566  
H -3.307299 -2.889912 -2.049372  
H -1.074442 -3.663460 -0.240627  
C -3.403823 0.546361 2.101505  
H -4.274350 0.926005 1.551202  
H -3.739649 -0.285534 2.721689  
H -3.000141 1.332751 2.743649  
Cl 2.283055 -2.171123 -1.730437

\*\*\*\*

LMZ TS2 2w

C 0.220616 0.888238 0.221285  
C -0.989446 1.445389 0.685821  
C 0.509395 -0.561860 0.345648  
C -2.508722 -0.473829 0.893971  
C -1.732805 -1.313534 0.012517  
O -3.715801 -0.714358 1.184400  
N -0.378087 -1.484209 0.195885  
N -1.916680 0.669183 1.451367  
C -1.252522 2.804378 0.450567  
C -0.334092 3.619426 -0.210339  
H -0.547300 4.671073 -0.372266  
C 0.862574 3.062077 -0.656534  
C 1.139457 1.715941 -0.447759  
H 2.075351 1.296129 -0.800524  
H -2.180010 3.244518 0.799913  
O -2.391782 -2.548950 -0.279590  
C 1.924746 -0.988437 0.573026  
C 2.621239 -0.457516 1.675310  
C 2.613031 -1.916089 -0.230684  
C 3.922603 -0.846158 1.985601  
H 2.110921 0.267705 2.304107  
C 3.918799 -2.314290 0.068311  
C 4.573462 -1.784246 1.180143  
H 4.423747 -0.421921 2.851450  
H 4.416906 -3.028817 -0.579342  
H 5.588635 -2.098896 1.406944  
H -2.360362 -0.801518 -1.520933  
Cl 2.036326 4.072503 -1.491736  
O -3.058284 -0.884049 -2.320048  
H -4.488950 -1.324703 0.024711  
H -2.066949 -3.220233 0.346560  
O -4.956153 -1.442018 -0.904126  
H -4.062195 -1.184105 -1.689942  
H -2.769779 -1.681954 -2.800078  
H -5.658774 -0.772129 -0.950332  
C -2.727546 1.372425 2.449981  
H -3.578399 1.913326 2.013703  
H -3.125857 0.642744 3.155680

H -2.082559 2.076131 2.981531  
Cl 1.891931 -2.582424 -1.692277

\*\*\*\*

LMZ TS4 0w

C -0.428362 0.469222 -0.272901  
C -1.785813 0.585565 0.150158  
C 0.251866 -0.828564 -0.391538  
C -2.767194 -1.719657 -0.059066  
C -1.839201 -1.942578 -1.272137  
O -3.601295 -2.515926 0.316732  
N -0.439096 -1.862950 -0.730259  
N -2.575133 -0.493476 0.613079  
C -2.340212 1.881196 0.202606  
C -1.613866 3.013689 -0.141387  
H -2.078217 3.993872 -0.101339  
C -0.284034 2.880068 -0.549565  
C 0.301148 1.626215 -0.609940  
H 1.333961 1.528846 -0.926647  
H -3.373347 2.000135 0.508903  
O -1.730138 -3.179273 -1.794418  
C 1.720513 -0.987407 -0.212342  
C 2.404056 -0.624029 0.961594  
C 2.462384 -1.552501 -1.264741  
C 3.783559 -0.800267 1.073243  
C 3.841375 -1.726124 -1.162972  
C 4.501765 -1.344718 0.007183  
H 4.283187 -0.521728 1.995345  
H 4.394524 -2.157661 -1.991830  
H 5.576205 -1.476425 0.099642  
Cl 0.642891 4.301464 -0.990576  
H -0.443105 -2.978042 -1.166004  
H -2.009468 -1.113183 -1.992600  
H 1.940170 -1.844701 -2.171502  
C -3.499569 -0.246944 1.731613  
H -4.480197 0.103515 1.386742  
H -3.649251 -1.190614 2.257096  
H -3.058756 0.488525 2.407107  
Cl 1.537396 0.000009 2.355165

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LMZ TS4 1w

C -0.126427 -0.779613 -0.284785  
C 0.786789 -1.756847 0.201175  
C 0.206583 0.650864 -0.334314  
C 2.990195 -0.581251 0.174750  
C 2.523299 0.147870 -1.122542  
O 4.096583 -0.451414 0.651442  
N 1.392982 1.045243 -0.651313  
N 2.038705 -1.436519 0.762239  
C 0.364245 -3.102160 0.213075  
C -0.892867 -3.481872 -0.237120  
H -1.183998 -4.527386 -0.228510  
C -1.778462 -2.508803 -0.711366  
C -1.404193 -1.175585 -0.727754  
H -2.098201 -0.425065 -1.090420  
H 1.044311 -3.866720 0.571750  
O 3.461690 0.873185 -1.735693

C -0.834823 1.694552 -0.109470  
C -1.603366 1.783789 1.064711  
C -1.052646 2.649344 -1.118761  
C -2.564904 2.782476 1.220139  
C -2.017426 3.644367 -0.974871  
C -2.775488 3.707696 0.196352  
H -3.133107 2.835985 2.142999  
H -2.173706 4.365510 -1.771583  
H -3.528140 4.480963 0.322344  
H 2.060496 -0.610995 -1.783116  
Cl -3.366238 -2.979659 -1.286706  
H 3.375747 2.032969 -1.323153  
H 1.786079 2.122257 -0.662672  
O 2.870477 3.017322 -0.824123  
H 2.789666 3.717762 -1.488653  
H -0.460832 2.590548 -2.027828  
C 2.517410 -2.220131 1.912150  
H 3.076437 -3.109762 1.597029  
H 3.191196 -1.588014 2.491144  
H 1.664773 -2.515925 2.526284  
Cl -1.333178 0.685299 2.407099

\*\*\*\*

LMZ TS4 2w

C -1.050544 -0.483742 -0.045477  
C -1.119544 -1.864438 0.292552  
C 0.207812 0.282899 0.016048  
C 1.261081 -2.581383 0.200289  
C 1.439861 -1.609500 -1.002276  
O 2.155375 -3.290243 0.622417  
N 1.331176 -0.238558 -0.344287  
N -0.015216 -2.595683 0.779050  
C -2.375789 -2.500264 0.227395  
C -3.521352 -1.820731 -0.164732  
H -4.472854 -2.339811 -0.220691  
C -3.439054 -0.464558 -0.496353  
C -2.223683 0.197500 -0.427724  
H -2.168159 1.251381 -0.677822  
H -2.450161 -3.553588 0.474337  
O 2.562586 -1.755997 -1.694007  
C 0.179967 1.679563 0.541244  
C -0.364233 1.901941 1.818883  
C 0.691167 2.786035 -0.161293  
C -0.370040 3.169902 2.394036  
H -0.769756 1.056568 2.367833  
C 0.673898 4.063414 0.402448  
C 0.152726 4.252546 1.682291  
H -0.780535 3.311656 3.389393  
H 1.065672 4.900110 -0.166570  
H 0.150103 5.248351 2.116720  
H 0.547909 -1.696242 -1.648102  
Cl -4.879468 0.399882 -0.996018  
H 3.594960 -1.690118 -1.035516  
H 2.359686 0.287523 -0.114642  
O 4.569072 -1.417853 -0.383341  
H 4.635641 -2.080216 0.321962  
O 3.588629 0.681937 0.312045  
H 3.948623 1.386664 -0.249074  
H 4.174988 -0.299949 0.055120

C -0.236728 -3.600610 1.830468  
H -0.489653 -4.581646 1.410415  
H 0.690079 -3.705018 2.395171  
H -1.039251 -3.263242 2.489394  
Cl 1.311964 2.624417 -1.795451

\*\*\*\*

XYZ coordinates for Table S9

ECF 1eq 0w

C 0.961922 -0.364408 0.528051  
 C 0.056715 -1.415792 0.291042  
 C 0.774950 0.976361 -0.090687  
 C -1.903477 -0.243851 -0.634582  
 C -1.531547 0.861530 0.368518  
 O -2.881462 -0.141312 -1.363266  
 N -0.371903 1.558347 -0.153403  
 N -0.993623 -1.299310 -0.688464  
 C 0.193600 -2.621578 0.989706  
 C 1.217772 -2.798719 1.912696  
 H 1.318319 -3.735445 2.450529  
 C 2.119178 -1.755160 2.137908  
 C 1.999302 -0.550903 1.457951  
 H 2.700185 0.254647 1.650258  
 H -0.499302 -3.431867 0.795393  
 C 1.951495 1.750731 -0.577848  
 C 1.973040 3.151250 -0.437308  
 C 3.047607 1.161683 -1.220647  
 C 3.047133 3.908914 -0.897329  
 H 1.120719 3.626142 0.037933  
 C 4.129906 1.894793 -1.692836  
 C 4.129379 3.279798 -1.523375  
 H 3.041335 4.987441 -0.769067  
 H 4.943017 1.375863 -2.190445  
 H 4.970452 3.864735 -1.885449  
 H -1.339202 0.396959 1.347314  
 Cl 3.414070 -1.966389 3.303813  
 F 3.058023 -0.179708 -1.431921  
 C -2.717926 1.818507 0.537216  
 O -2.806444 2.930745 0.077763  
 O -3.651082 1.225427 1.308710  
 C -4.884501 1.963117 1.509843  
 H -5.320776 2.172069 0.528168  
 H -4.641668 2.918924 1.984858  
 C -5.794801 1.109597 2.372335  
 H -6.739705 1.638469 2.543424  
 H -6.018325 0.155458 1.883366  
 H -5.336423 0.902505 3.345493  
 C -0.991221 -2.328985 -1.733543  
 N -2.024052 -2.305967 -2.596893  
 H -2.717747 -1.570200 -2.498733  
 O -0.077126 -3.139826 -1.773359  
 C -2.066958 -3.249079 -3.705785  
 H -2.986681 -3.069207 -4.266655  
 H -1.206033 -3.118800 -4.370463  
 H -2.063006 -4.280316 -3.338889

\*\*\*\*

ECF 1eq 1w

C -1.024613 -0.546088 -0.521268  
 C -0.187275 -1.613597 -0.145754  
 C -0.757096 0.851347 -0.086270  
 C 1.853083 -0.459699 0.604575  
 C 1.534170 0.531624 -0.529636  
 O 2.851766 -0.327053 1.299474

N 0.426378 1.366430 -0.092723  
 N 0.881180 -1.436444 0.803856  
 C -0.413276 -2.891349 -0.671718  
 C -1.459941 -3.123665 -1.556678  
 H -1.628937 -4.116300 -1.960377  
 C -2.294686 -2.063244 -1.918359  
 C -2.086807 -0.788336 -1.409686  
 H -2.736635 0.028186 -1.706096  
 H 0.226792 -3.712457 -0.371027  
 C -1.895284 1.734800 0.286004  
 C -1.917864 3.080717 -0.122950  
 C -2.965757 1.290115 1.073771  
 C -2.969527 3.923644 0.228578  
 H -1.092036 3.456940 -0.717263  
 C -4.023670 2.110652 1.440786  
 C -4.024116 3.438250 1.008123  
 H -2.959948 4.959032 -0.097846  
 H -4.815881 1.707341 2.063425  
 H -4.844784 4.092594 1.288940  
 H 1.293747 -0.035764 -1.439913  
 Cl -3.616515 -2.344110 -3.036813  
 F -2.965081 0.012696 1.534720  
 C 2.784288 1.367975 -0.823031  
 O 2.981629 2.503817 -0.459150  
 O 3.635471 0.641475 -1.566000  
 C 4.920264 1.251976 -1.865716  
 H 5.404803 1.504948 -0.917872  
 H 4.738650 2.180396 -2.415972  
 C 5.724672 0.252686 -2.674437  
 H 6.703273 0.682592 -2.917454  
 H 5.885866 -0.671475 -2.109457  
 H 5.216807 0.003537 -3.612376  
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 H 2.603472 -1.566011 2.633020  
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 C 1.857698 -3.012303 4.064421  
 H 2.793814 -2.818144 4.592253  
 H 1.015266 -2.728151 4.704221  
 H 1.778911 -4.082342 3.848799  
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 H 1.948502 4.267505 0.949188  
 H 0.821765 3.274283 0.746263

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ECF 1eq 2w

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 C -0.646161 -1.639173 0.165595  
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 C 1.598286 -0.693791 0.449634  
 C 1.319175 -0.022273 -0.903519  
 O 2.660807 -0.506682 1.044759  
 N 0.424214 1.086757 -0.636268  
 N 0.539115 -1.421115 0.960558  
 C -1.115987 -2.947189 0.001641  
 C -2.276944 -3.199719 -0.720433  
 H -2.636976 -4.215313 -0.845845  
 C -2.976830 -2.128250 -1.281287  
 C -2.525608 -0.823819 -1.129646

H -3.073619 -0.002592 -1.579208  
 H -0.576219 -3.769835 0.455730  
 C -1.713119 1.984635 -0.134745  
 C -1.439236 3.224291 -0.744274  
 C -2.815714 1.933496 0.729041  
 C -2.245332 4.335679 -0.517718  
 H -0.570047 3.294609 -1.388965  
 C -3.634801 3.028473 0.973466  
 C -3.347789 4.237365 0.338383  
 H -2.008551 5.279330 -0.999740  
 H -4.467537 2.922517 1.661402  
 H -3.979197 5.102371 0.521828  
 H 0.893020 -0.765882 -1.592428  
 Cl -4.439782 -2.435794 -2.198507  
 F -3.093697 0.782223 1.395547  
 C 2.634920 0.475385 -1.508528  
 O 3.036936 1.616749 -1.484901  
 O 3.281199 -0.551708 -2.082214  
 C 4.586125 -0.263071 -2.656571  
 H 5.224408 0.140204 -1.864510  
 H 4.460305 0.510462 -3.420190  
 C 5.130317 -1.556417 -3.231255  
 H 6.116528 -1.372881 -3.672968  
 H 5.238900 -2.318925 -2.452719  
 H 4.471750 -1.948636 -4.013542  
 C 0.473718 -1.944362 2.338814  
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 H 0.808824 -1.665994 5.052438  
 H 1.372082 -3.279519 4.571804  
 O 2.262109 3.934098 0.433605  
 H 2.257154 3.285134 -0.291055  
 H 2.549984 3.405712 1.202144  
 O 3.584030 2.000452 2.248822  
 H 4.468393 2.275829 1.963608  
 H 3.385854 1.191746 1.741530

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ECF TS2 0w

C -0.426190 -0.506925 0.456900  
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 C 2.141167 0.358806 -0.806510  
 C 1.191077 1.477508 -0.919348  
 O 3.141510 0.614464 -1.589279  
 N -0.136714 1.196441 -1.301793  
 N 1.955158 -0.815044 -0.191913  
 C 1.193363 -1.412707 2.040991  
 C 0.207028 -1.561034 3.008979  
 H 0.446746 -1.962523 3.987540  
 C -1.100374 -1.188150 2.693119  
 C -1.416721 -0.668644 1.444713  
 H -2.436399 -0.367070 1.233078  
 H 2.211880 -1.713911 2.260201  
 C -2.178279 0.003849 -1.359735  
 C -2.951660 1.092089 -1.803722

C -2.726229 -1.271654 -1.533675  
C -4.212158 0.903675 -2.366495  
H -2.533193 2.087856 -1.695729  
C -3.978214 -1.490073 -2.096455  
C -4.728710 -0.389259 -2.511766  
H -4.792296 1.762927 -2.691011  
H -4.338684 -2.507853 -2.208080  
H -5.710566 -0.543284 -2.950942  
Cl -2.364831 -1.366671 3.897648  
H 2.407859 1.564305 -1.891051  
F -2.000774 -2.361586 -1.164530  
C 1.511304 2.696439 -0.149991  
O 0.522982 3.616274 -0.238792  
O 2.550565 2.868294 0.473919  
C 0.742449 4.879958 0.436632  
H 0.153471 5.594582 -0.144409  
H 1.801819 5.139414 0.367964  
C 0.277213 4.824742 1.884600  
H 0.876061 4.112272 2.460069  
H 0.386232 5.814709 2.345027  
H -0.777120 4.532749 1.945425  
C 2.676012 -2.072052 -0.492302  
O 2.204057 -3.124848 -0.104464  
N 3.832714 -1.935483 -1.165655  
H 4.113614 -1.015187 -1.486844  
C 4.576247 -3.119501 -1.581461  
H 4.001064 -3.719251 -2.295263  
H 5.504971 -2.788921 -2.050692  
H 4.810349 -3.744514 -0.715070

\*\*\*\*

ECF TS2 1w

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C 1.747694 -0.817809 0.198253  
C 1.473138 0.569703 -0.075514  
O 2.864528 -1.359512 -0.028374  
N 0.322651 1.231451 0.361899  
N 0.659762 -1.615883 0.670594  
C -0.870594 -2.837294 -0.801401  
C -2.010552 -2.898878 -1.595485  
H -2.296305 -3.825640 -2.082096  
C -2.788702 -1.748158 -1.754146  
C -2.445078 -0.558922 -1.126054  
H -3.060749 0.323940 -1.259270  
H -0.268655 -3.727009 -0.650203  
C -1.965127 1.701759 0.795353  
C -2.952223 1.209404 1.667502  
C -2.032163 3.062367 0.468831  
C -3.935467 2.041828 2.202296  
H -2.928356 0.156863 1.937659  
C -3.005817 3.912030 0.981248  
C -3.960858 3.397133 1.860119  
H -4.676214 1.634538 2.884548  
H -3.005859 4.955677 0.682283  
H -4.723783 4.053568 2.269808  
H 1.727158 0.038471 -1.722007  
Cl -4.225427 -1.810330 -2.765899

O 2.475614 -0.341264 -2.432331  
H 2.831466 -1.066424 -1.833342  
H 3.147083 0.387947 -2.261680  
F -1.147624 3.587781 -0.414602  
C 2.659326 1.508613 0.049751  
O 2.803084 2.334977 0.914473  
O 3.603020 1.394840 -0.968664  
C 4.785550 2.236916 -0.845414  
H 5.263378 2.005912 0.110230  
H 4.458791 3.279720 -0.822898  
C 5.692139 1.942849 -2.025973  
H 6.592248 2.564094 -1.956612  
H 6.009116 0.893657 -2.035947  
H 5.200486 2.176076 -2.977990  
C 0.793968 -2.604221 1.690126  
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H 2.822971 -2.429148 1.665949  
C 2.262075 -3.713196 3.287777  
H 1.535185 -3.558229 4.088621  
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H 3.268782 -3.558256 3.684339  
O -0.191042 -3.221620 2.082207

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ECF TS2 2w

C -1.319336 -0.651176 -0.281129  
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C 1.724425 -0.601912 0.348781  
C 1.332907 0.667938 -0.110666  
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N 0.125428 1.277193 0.199886  
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C -1.760496 -3.224501 -1.345451  
H -1.947742 -4.216986 -1.741963  
C -2.645711 -2.176980 -1.616360  
C -2.440360 -0.906646 -1.093929  
H -3.141774 -0.108835 -1.313451  
H 0.028276 -3.781014 -0.288911  
C -2.201095 1.570322 0.611197  
C -3.149835 1.064996 1.518642  
C -2.389848 2.887565 0.171170  
C -4.212999 1.843672 1.976137  
H -3.032254 0.045824 1.877737  
C -3.444511 3.682352 0.605820  
C -4.359555 3.157132 1.520613  
H -4.921244 1.427270 2.686896  
H -3.537551 4.692463 0.218838  
H -5.185061 3.771873 1.869208  
H 3.333166 -0.934063 -3.370001  
Cl -4.048321 -2.477653 -2.635594  
O 3.931844 -0.881135 -2.607614  
H 3.424982 -2.110436 -0.260804  
O 3.860351 -2.705651 -1.029707  
H 3.893408 -1.855412 -1.920519  
H 3.647992 -0.040778 -2.030988  
H 3.271295 -3.452245 -1.224423  
F -1.546989 3.419998 -0.747240

C 2.343574 1.559057 -0.685725  
O 3.331078 1.208025 -1.369809  
O 2.116865 2.854270 -0.467747  
C 3.013151 3.827188 -1.059674  
H 2.389685 4.718369 -1.164712  
H 3.318982 3.476480 -2.048446  
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H 4.828437 4.888777 -0.599605  
H 3.891735 4.412042 0.833032  
H 4.833841 3.194934 -0.064144  
C 0.749562 -2.145659 2.088973  
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H 2.674683 -1.536558 2.383132  
C 2.008164 -2.586809 4.132862  
H 1.122687 -2.407549 4.747936  
H 2.139887 -3.672198 4.033018  
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O -0.195566 -2.840414 2.454945

\*\*\*\*

XYZ coordinates for Table S10

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	H 0.077626 5.207894 0.717297	C -2.689574 -0.040891 0.295821
	H 2.245393 5.501027 -0.471738	O -3.853540 -1.926839 -0.580454
	H -0.647924 -2.408503 -2.468534	N -1.678882 0.863122 0.227069
C 0.292914 -0.599250 -0.040236	H -1.558239 -1.291917 0.792454	N -1.681762 -1.680461 -1.233357
C -0.224973 -1.719907 -0.729471	Cl 4.255578 -1.709210 1.682777	C 0.266292 -3.012845 -0.657610
C -0.485734 0.665799 0.088045	H -0.963633 2.956899 0.863228	C 1.568710 -3.150427 -0.175520
C -2.690227 -1.266745 -0.734701	C -3.419835 -0.425465 0.429302	H 2.073735 -4.110982 -0.194385
C -2.463341 -0.527115 0.603880	N -4.502406 -0.259585 0.804669	C 2.193550 -2.021535 0.347938
O -3.770593 -1.442461 -1.258538	O -7.337729 0.099091 1.907919	C 1.556506 -0.786041 0.368773
N -1.746114 0.716698 0.356082	H -7.881683 0.049043 1.108373	H 2.068663 0.070693 0.791570
N -1.510544 -1.714069 -1.304421	H -6.420794 -0.002098 1.593972	H -0.251070 -3.885628 -1.051333
C 0.575862 -2.862473 -0.899103	****	C 0.389317 1.943177 -0.172805
C 1.858993 -2.923701 -0.370736	CNZ 1eq 2w	C 1.537390 2.035096 -0.986420
H 2.466066 -3.813702 -0.500281		C -0.016149 3.109984 0.510316
C 2.351437 -1.831871 0.351747	C 1.228099 -0.422223 -0.085414	C 2.251983 3.230106 -1.103507
C 1.587757 -0.682767 0.506676	C 1.550673 -1.668264 -0.671719	H 1.864616 1.165059 -1.549369
H 1.992045 0.164602 1.049332	C -0.100199 0.222152 -0.295161	C 0.700366 4.299414 0.398689
H 0.175891 -3.716496 -1.439933	C -0.701155 -2.642603 -1.179956	C 1.843807 4.371978 -0.408539
C 0.216301 1.968037 -0.105408	C -1.213723 -1.838254 0.033383	H 3.129126 3.267476 -1.747226
C 1.310104 2.092477 -0.979067	O -1.376247 -3.405173 -1.842131	H 0.365135 5.178716 0.946039
C -0.253358 3.112119 0.563858	N -1.220969 -0.417491 -0.281152	H 2.401210 5.302116 -0.496934
C 1.919865 3.332633 -1.178994	N 0.628432 -2.390643 -1.457350	H -1.956909 -2.531076 -1.715972
H 1.675196 1.225164 -1.521234	C 2.844508 -2.194883 -0.518932	Cl 3.835410 -2.164176 1.005656
C 0.364506 4.346295 0.371611	C 3.806134 -1.528096 0.229449	H -0.913057 3.058887 1.119447
C 1.452801 4.460972 -0.500587	H 4.799821 -1.947414 0.348348	C -3.880283 0.427255 0.934752
H 2.757671 3.415663 -1.866201	C 3.470764 -0.319638 0.848640	N -4.822492 0.827600 1.500762
H -0.002906 5.220501 0.902508	C 2.207123 0.232434 0.686518	****
H 1.932258 5.424741 -0.651087	H 1.967924 1.181726 1.152746	CNZ An1 1w
H -1.661540 -2.305754 -2.115364	H 3.089485 -3.147386 -0.982157	C 0.848046 -0.593659 -0.187983
H -1.888852 -1.205198 1.259055	C -0.165095 1.691096 -0.534004	C 0.440087 -1.832992 -0.731872
Cl 3.955097 -1.912337 1.057207	C 0.865586 2.371821 -1.206839	C -0.025068 0.609506 -0.209659
H -1.105005 3.017213 1.229576	C -1.301167 2.407126 -0.113047	C -2.038536 -1.697991 -0.811823
C -3.742165 -0.248679 1.276328	C 0.763046 3.741443 -1.455487	C -2.181274 -0.464347 -0.075701
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****	C -1.390670 3.778167 -0.351876	N -1.320187 0.590186 -0.056616
CNZ 1eq 1w	C -0.362615 4.448742 -1.023207	N -0.777060 -1.948289 -1.439357
	H 1.560964 4.253592 -1.986887	C 1.278281 -2.953948 -0.628458
C 0.802826 -0.590168 -0.095311	H -2.269116 4.317882 -0.008848	C 2.523626 -2.884095 -0.003591
C 0.476326 -1.741205 -0.848660	H -0.437599 5.517290 -1.208957	H 3.168650 -3.754934 0.055669
C -0.044200 0.636092 -0.132295	H 1.005479 -2.995230 -2.180464	C 2.906597 -1.669163 0.558704
C -1.962205 -1.413251 -1.318943	H -0.555674 -2.070800 0.889209	C 2.088911 -0.547503 0.480049
C -2.022674 -0.648883 0.024356	Cl 4.663978 0.510609 1.828933	H 2.413579 0.381595 0.934335
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H 3.173546 -3.695706 -0.088025	H -5.020780 -1.328420 1.641202	H 2.290090 1.405478 -1.474459
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C 1.976510 -0.603761 0.682684	H -4.678692 1.619672 -0.154401	C 1.698328 4.576255 -0.388155
H 2.232231 0.267167 1.275943	H -4.849636 1.058856 1.270353	H 3.248414 3.670768 -1.588744
H 1.096337 -3.721146 -1.437667	****	H 0.001013 5.160959 0.815325
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C 2.422484 3.410523 -0.975862	C -0.393033 -1.773995 -0.662041	H -0.966449 2.877829 0.903408
H 2.339655 1.293261 -1.335964		
C 0.572305 4.351633 0.266664		

C -3.492644 -0.181692 0.404692  
N -4.548991 0.064612 0.841288  
O -7.431832 0.282977 1.248349  
H -7.667968 -0.371227 0.574547  
H -6.449129 0.293477 1.216965

\*\*\*\*

CNZ An1 2w

C 0.951651 -0.542509 -0.345412  
C 0.484137 -1.701489 -1.003799  
C 0.180838 0.730824 -0.329363  
C -1.969507 -1.345835 -1.235436  
C -2.053388 -0.172943 -0.391385  
O -2.936608 -2.025841 -1.597359  
N -1.114430 0.816162 -0.262047  
N -0.694057 -1.675858 -1.781606  
C 1.229577 -2.889425 -0.942600  
C 2.434511 -2.962915 -0.245708  
H 3.005665 -3.885287 -0.215115  
C 2.874039 -1.826626 0.429077  
C 2.149306 -0.641166 0.390400  
H 2.513743 0.224574 0.931407

H 0.855580 -3.772875 -1.455992  
C 0.916840 2.027215 -0.245220  
C 2.157260 2.225239 -0.881759  
C 0.348172 3.122454 0.435770  
C 2.805656 3.462310 -0.835292  
H 2.611868 1.407026 -1.433892  
C 0.998364 4.353700 0.489167  
C 2.234126 4.534743 -0.145456  
H 3.759200 3.586557 -1.344966  
H 0.539273 5.178476 1.030814  
H 2.740065 5.496896 -0.104485  
H -0.816620 -2.512844 -2.343698  
Cl 4.383266 -1.894319 1.353539  
H -0.617451 2.985487 0.912022  
C -3.374690 0.205206 -0.013176  
N -4.438036 0.506137 0.370916  
O -7.310582 0.670364 0.887426  
H -7.558885 -0.024588 0.260374  
H -6.334156 0.724243 0.791186  
O -2.285542 -1.592372 2.720665  
H -3.208141 -1.430636 2.971332  
H -2.219510 -1.188594 1.835310

\*\*\*\*

CNZ An2 0w

C 0.300733 -0.621462 -0.040121  
C -0.208951 -1.819725 -0.659292  
C -0.534542 0.587130 0.095340  
C -2.558045 -1.422327 -0.831375  
C -2.445455 -0.688086 0.577805  
O -3.642564 -1.429151 -1.417372  
N -1.803755 0.587761 0.355017  
N -1.420759 -1.998228 -1.240607  
C 0.706397 -2.917999 -0.764120  
C 2.001596 -2.868305 -0.292159  
H 2.660308 -3.727624 -0.383797

C 2.462974 -1.685788 0.314130  
C 1.638701 -0.584869 0.424639  
H 2.013454 0.320286 0.891810  
H 0.329379 -3.815706 -1.246121  
C 0.082589 1.942269 -0.087745  
C 1.120493 2.165263 -1.007869  
C -0.417291 3.039928 0.634290  
C 1.645313 3.446243 -1.198701  
H 1.507426 1.332981 -1.588333  
C 0.111312 4.317800 0.450597  
C 1.147064 4.527528 -0.466898  
H 2.442284 3.597938 -1.923491  
H -0.286166 5.152815 1.023800  
H 1.558999 5.524081 -0.611503  
Cl 4.122576 -1.621120 0.944718  
H -1.232443 2.870842 1.330892  
C -3.753219 -0.494435 1.221123  
N -4.759447 -0.370778 1.789121  
H -1.846797 -1.333647 1.242940

\*\*\*\*

CNZ An2 1w

C -0.749250 -0.631866 0.080577  
C -0.225697 -1.792770 0.754861  
C 0.014869 0.628485 0.013807  
C 2.066900 -1.251785 1.144113  
C 2.037711 -0.522589 -0.275342  
O 3.097333 -1.192947 1.819382  
N 1.300412 0.710054 -0.126255  
N 0.934806 -1.890538 1.452078  
C -1.071926 -2.948470 0.780256  
C -2.315552 -2.985188 0.184206  
H -2.922139 -3.885997 0.218342  
C -2.792193 -1.836985 -0.473647  
C -2.035421 -0.683979 -0.511937  
H -2.421596 0.193909 -1.020037  
H -0.685690 -3.818339 1.304029  
C -0.702745 1.940584 0.125412  
C -1.834270 2.097013 0.943112  
C -0.210375 3.066081 -0.557663  
C -2.457170 3.341123 1.072204  
H -2.218254 1.242975 1.493084  
C -0.836272 4.306847 -0.435776  
C -1.964300 4.450438 0.379792  
H -3.326500 3.442328 1.718210  
H -0.442703 5.164249 -0.977560  
H -2.452070 5.418064 0.476254  
Cl -4.382018 -1.882872 -1.262487  
H 0.674707 2.949455 -1.175148  
C 3.391926 -0.245154 -0.770610  
N 4.453651 -0.062041 -1.202505  
H 1.556581 -1.206546 -0.995241  
O 7.416683 -0.062164 -1.045331  
H 6.458432 -0.010327 -1.239890  
H 7.441918 -0.333092 -0.115575

\*\*\*\*

CNZ An2 2w

C -0.939882 -0.592802 -0.130612  
C -0.274796 -1.785602 0.318914  
C -0.284906 0.728499 -0.055734  
C 1.989120 -1.108482 0.596698  
C 1.787509 -0.182704 -0.671037  
O 3.083048 -1.065244 1.186761  
N 0.972706 0.945628 -0.275280  
N 0.949890 -1.871930 0.908424  
C -1.017566 -3.004140 0.234635  
C -2.299442 -3.067226 -0.273499  
H -2.828189 -4.014461 -0.331496  
C -2.917638 -1.885072 -0.716768  
C -2.262038 -0.673574 -0.632481  
H -2.757720 0.230041 -0.972303  
H -0.522461 -3.900526 0.596865  
C -1.092610 1.937207 0.310479  
C -2.151846 1.865576 1.230225  
C -0.758454 3.189999 -0.231698  
C -2.858491 3.013953 1.596491  
H -2.412211 0.908954 1.673444  
C -1.469639 4.335420 0.126367  
C -2.524051 4.252531 1.042538  
H -3.668655 2.939029 2.318319  
H -1.199996 5.295096 -0.309081  
H -3.077658 5.145783 1.323551  
Cl -4.556839 -1.960606 -1.389848  
H 0.071675 3.247660 -0.928737  
C 3.066718 0.290451 -1.218809  
N 4.060658 0.641561 -1.703438  
H 1.298318 -0.785861 -1.455040  
O 6.875277 1.224443 -2.474203  
H 5.916759 1.095864 -2.321312  
H 7.287612 0.821624 -1.696007  
O 4.166656 -2.169834 3.519001  
H 3.621707 -1.916984 2.735788  
H 4.902534 -1.541871 3.478740

\*\*\*\*

CNZ TS2 0w

C -0.224672 0.518257 -0.199125  
C -1.366542 1.065732 -0.817860  
C 0.055859 -0.951974 -0.024573  
C -2.833509 -0.865314 -0.783943  
C -2.207887 -1.628240 0.313560  
O -3.837435 -1.532023 -1.232271  
N -0.804207 -1.857029 0.295912  
N -2.374504 0.229698 -1.379841  
C -1.541627 2.448385 -0.925426  
C -0.601619 3.328333 -0.397636  
H -0.739668 4.401226 -0.477470  
C 0.511096 2.799927 0.256937  
C 0.701219 1.424618 0.351548  
H 1.580985 1.043683 0.856677  
H -2.431470 2.838173 -1.413130  
C 1.480519 -1.400147 -0.123562  
C 1.938113 -2.445677 0.696995  
C 2.362810 -0.841692 -1.063354  
C 3.248465 -2.908379 0.588957  
H 1.252518 -2.886796 1.413300

C 3.670925 -1.317548 -1.181537  
C 4.119633 -2.347965 -0.352061  
H 3.591268 -3.708766 1.239584  
H 4.337103 -0.881989 -1.921772  
H 5.139955 -2.712692 -0.437704  
H -2.834547 0.526754 -2.236104  
Cl 1.694078 3.883214 0.963360  
H -3.341052 -2.382582 -0.452665  
H 2.025215 -0.042194 -1.717441  
C -2.830302 -1.543117 1.600322  
N -3.332010 -1.510448 2.654262

\*\*\*\*

CNZ TS2 1w

C 0.368866 -0.618092 -0.202284  
C -0.463556 -1.532857 -0.873286  
C 0.043202 0.835373 -0.092157  
C -2.692998 -0.485832 -0.757584  
C -2.358151 0.645679 0.100093  
O -3.867453 -0.934697 -0.832778  
N -1.132647 1.333157 0.064523  
N -1.696255 -1.145903 -1.469546  
C -0.087479 -2.880096 -0.974171  
C 1.091308 -3.345931 -0.398269  
H 1.374168 -4.389683 -0.486599  
C 1.890900 -2.450184 0.310723  
C 1.540746 -1.107547 0.403706  
H 2.184286 -0.423121 0.944434  
H -0.730144 -3.576314 -1.508219  
C 1.172283 1.817865 -0.119787  
C 2.300304 1.619361 -0.934373  
C 1.086552 3.001822 0.633251  
C 3.314842 2.577700 -0.993827  
H 2.379577 0.722180 -1.541888  
C 2.106202 3.951200 0.584354  
C 3.224960 3.743908 -0.230225  
H 4.173384 2.412060 -1.639721  
H 2.027413 4.856288 1.181379  
H 4.017739 4.486520 -0.270606  
H -2.125355 -1.901320 -1.997609  
H -3.046631 -0.218285 1.366739  
Cl 3.362081 -3.020076 1.083722  
O -3.972676 -0.772517 1.697440  
H -4.282408 -0.961640 0.725146  
H -4.569828 -0.084424 2.055548  
H 0.207704 3.166507 1.248419  
C -3.467146 1.560735 0.284562  
N -4.380990 2.228690 0.567603

\*\*\*\*

CNZ TS2 2w

C -0.554924 0.613756 -0.293269  
C 0.373006 1.364484 -1.039014  
C -0.464339 -0.872011 -0.178381  
C 2.395076 -0.056756 -1.079903  
C 1.939662 -1.024412 -0.102413  
O 3.600062 0.109921 -1.396613  
N 0.630688 -1.539663 -0.062949

N 1.450470 0.747203 -1.724998  
C 0.229873 2.756561 -1.137600  
C -0.805667 3.423467 -0.487708  
H -0.911294 4.499850 -0.575343  
C -1.694125 2.683972 0.292618  
C -1.576937 1.301308 0.386408  
H -2.289724 0.742376 0.982074  
H 0.940108 3.325725 -1.733346  
C -1.732693 -1.663611 -0.127098  
C -2.871065 -1.279851 -0.856639  
C -1.785322 -2.853046 0.621280  
C -4.029255 -2.060974 -0.837176  
H -2.848815 -0.376260 -1.459389  
C -2.945514 -3.624887 0.650972  
C -4.073734 -3.232842 -0.078571  
H -4.895040 -1.752422 -1.417776  
H -2.969943 -4.536378 1.243163  
H -4.976987 -3.837306 -0.057332  
H 1.929723 1.369014 -2.369461  
H 2.491191 -0.137510 1.336187  
Cl -2.985356 3.506798 1.157032  
O 3.144595 0.235497 2.087769  
H 4.701790 0.252356 -0.215310  
O 5.122357 0.513233 0.672856  
H 4.106419 0.412663 1.517706  
H 3.296400 -0.514494 2.695167  
H 5.469234 1.414481 0.572983  
H -0.901473 -3.163716 1.169266  
C 2.927418 -2.021791 0.231094  
N 3.730926 -2.765161 0.636829

\*\*\*\*

XYZ coordinates for Table S11

ELZ 1eq 0w

C -0.834562 -0.719951 0.111683  
C -0.181291 -1.646519 0.954688  
C -0.423185 0.710074 0.057971  
C 1.984124 -0.485095 1.451906  
C 1.873559 0.162181 0.057871  
O 2.916776 -0.328171 2.218078  
N 0.793950 1.124825 0.054808  
N 0.896956 -1.274772 1.779529  
C -0.652520 -2.968161 1.029299  
C -1.735259 -3.388238 0.267080  
H -2.087633 -4.412688 0.327347  
C -2.354836 -2.477646 -0.594286  
C -1.920772 -1.161572 -0.665174  
H -2.429518 -0.460155 -1.318057  
H -0.152053 -3.673983 1.687523  
C -1.477412 1.764519 -0.047474  
C -1.273309 2.872725 -0.889556  
C -2.664391 1.745046 0.694090  
C -2.223533 3.886038 -0.998321  
H -0.345597 2.919966 -1.450872  
C -3.626575 2.743774 0.609859  
C -3.404013 3.820107 -0.250471  
H -2.043018 4.726526 -1.662163  
H -4.520512 2.671200 1.221193  
H -4.148836 4.607362 -0.328328  
H 1.020967 -1.789219 2.645718  
H 1.702065 -0.651462 -0.665624  
Cl -3.703377 -3.004796 -1.587243  
F -2.889679 0.727492 1.569191  
C 3.206925 0.830681 -0.295196  
O 3.444562 2.012540 -0.240744  
O 4.082805 -0.115694 -0.687975  
C 5.437098 0.331698 -0.954317  
H 5.814311 0.829662 -0.055947  
H 5.405238 1.067365 -1.764344  
C 6.259406 -0.889278 -1.320961  
H 7.292526 -0.587162 -1.529045  
H 6.271382 -1.614195 -0.500199  
H 5.858989 -1.381194 -2.214183

\*\*\*\*

ELZ 1eq 1w

C -0.875821 -0.591177 -0.205871  
C -0.149803 -1.642097 0.399869  
C -0.529595 0.835341 0.037946  
C 1.976258 -0.515721 1.060410  
C 1.786207 0.422326 -0.147240  
O 2.943135 -0.487853 1.807923  
N 0.666021 1.305945 0.093129  
N 0.947687 -1.410362 1.243609  
C -0.570178 -2.971594 0.214150  
C -1.666859 -3.271209 -0.583501  
H -1.978328 -4.300669 -0.727722  
C -2.357077 -2.230344 -1.213284  
C -1.979127 -0.910016 -1.019110

H -2.543353 -0.111997 -1.490324  
H -0.017739 -3.771021 0.700278  
C -1.634147 1.831517 0.194019  
C -1.524197 3.096753 -0.410351  
C -2.780443 1.596592 0.961801  
C -2.524486 4.057184 -0.271777  
H -0.628849 3.307767 -0.986410  
C -3.790677 2.536868 1.122389  
C -3.661723 3.776032 0.492800  
H -2.416275 5.023373 -0.756114  
H -4.648822 2.292405 1.740482  
H -4.445098 4.520248 0.607380  
H 1.148419 -2.103261 1.972366  
H 1.621804 -0.216470 -1.030248  
Cl -3.726398 -2.601251 -2.250499  
F -2.914761 0.412305 1.618869  
C 3.073605 1.219781 -0.376937  
O 3.272726 2.361667 -0.040265  
O 3.964247 0.442686 -1.027385  
C 5.283942 1.008216 -1.228976  
H 5.694900 1.272989 -0.249801  
H 5.181856 1.927287 -1.814920  
C 6.125957 -0.033849 -1.940979  
H 7.135199 0.360532 -2.108110  
H 6.207959 -0.947425 -1.342531  
H 5.693340 -0.293343 -2.913456  
O 1.522526 -3.392868 3.326227  
H 2.427888 -3.108966 3.537094  
H 1.020679 -3.286664 4.149404

\*\*\*\*

ELZ 1eq 2w

C -1.029583 -0.537416 -0.374245  
C -0.169342 -1.592479 0.007276  
C -0.758805 0.874214 0.010676  
C 1.902732 -0.376833 0.623201  
C 1.539770 0.657858 -0.454608  
O 2.918863 -0.283964 1.313089  
N 0.402259 1.428188 0.001341  
N 1.002005 -1.391541 0.762135  
C -0.518501 -2.917465 -0.307796  
C -1.673852 -3.205584 -1.021548  
H -1.929497 -4.231363 -1.266100  
C -2.499861 -2.154715 -1.433211  
C -2.193383 -0.842861 -1.104353  
H -2.860144 -0.041436 -1.404692  
H 0.133061 -3.723622 0.015787  
C -1.902653 1.755049 0.398471  
C -1.937197 3.089576 -0.044729  
C -2.943719 1.340541 1.237374  
C -2.975899 3.946407 0.314016  
H -1.123506 3.437384 -0.673152  
C -3.988417 2.174662 1.616112  
C -4.005259 3.487734 1.143052  
H -2.981407 4.970016 -0.049219  
H -4.758847 1.791640 2.277849  
H -4.817449 4.150533 1.428798  
H 1.282288 -2.163268 1.389233  
H 1.318778 0.107318 -1.383030

Cl -3.947709 -2.504143 -2.363884  
F -2.931784 0.078208 1.743248  
C 2.745903 1.564537 -0.722049  
O 2.893879 2.690528 -0.313651  
O 3.625511 0.905961 -1.503799  
C 4.877339 1.585446 -1.778911  
H 5.354468 1.822530 -0.823006  
H 4.654342 2.527040 -2.290880  
C 5.725779 0.658531 -2.628764  
H 6.682215 1.143076 -2.857566  
H 5.932409 -0.278599 -2.101047  
H 5.225829 0.422139 -3.574440  
O 3.644831 -1.776293 3.536287  
H 3.480055 -1.160919 2.783449  
H 3.544740 -1.252963 4.345060  
O 1.759985 -3.489092 2.592586  
H 2.451854 -2.990874 3.097770  
H 2.163205 -4.338914 2.361770

\*\*\*\*

ELZ An1 0w

C -1.366937 -0.581860 0.187121  
C -1.378354 -1.943790 0.570186  
C -0.160363 0.257979 0.356701  
C 1.053232 -2.584203 0.766762  
C 1.634474 -1.372632 0.214601  
O 1.627619 -3.654370 0.982080  
N 1.075626 -0.140845 0.285657  
N -0.295034 -2.500609 1.274977  
C -2.520862 -2.723925 0.334720  
C -3.670932 -2.187442 -0.249803  
H -4.553267 -2.799080 -0.409571  
C -3.648350 -0.848948 -0.630407  
C -2.521578 -0.058380 -0.428174  
H -2.534167 0.980739 -0.738266  
H -2.514321 -3.770292 0.634274  
C -0.353260 1.732307 0.509778  
C -1.206769 2.252933 1.503677  
C 0.318605 2.686798 -0.271402  
C -1.359690 3.623515 1.717395  
H -1.748860 1.546784 2.128094  
C 0.190408 4.058706 -0.079390  
C -0.653113 4.536204 0.927394  
H -2.021766 3.977037 2.504672  
H 0.742637 4.731957 -0.729259  
H -0.758614 5.606975 1.085238  
H -0.505482 -3.420401 1.651161  
Cl -5.084635 -0.137283 -1.394673  
F 1.108537 2.285388 -1.299058  
C 3.037092 -1.422538 -0.219310  
O 3.678678 -2.416154 -0.540287  
O 3.615282 -0.170096 -0.291384  
C 4.952416 -0.140549 -0.788311  
H 4.986656 -0.594631 -1.786995  
H 5.605835 -0.739093 -0.140206  
C 5.390565 1.316602 -0.825280  
H 6.417088 1.393722 -1.208787  
H 4.729583 1.904027 -1.472362  
H 5.360359 1.758040 0.177721



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ELZ An1 1w

C 1.365547 -0.774243 -0.196217  
 C 0.963774 -2.064953 -0.606763  
 C 0.482652 0.401626 -0.380491  
 C -1.534131 -1.916019 -0.857120  
 C -1.725300 -0.602920 -0.278531  
 O -2.407279 -2.756600 -1.115732  
 N -0.812807 0.406725 -0.337520  
 N -0.222728 -2.246001 -1.343013  
 C 1.799957 -3.165034 -0.363879  
 C 3.040822 -3.018356 0.260042  
 H 3.684371 -3.875932 0.428616  
 C 3.425176 -1.744528 0.669227  
 C 2.606301 -0.640151 0.455555  
 H 2.931450 0.340547 0.785220  
 H 1.477696 -4.153859 -0.684116  
 C 1.132538 1.741816 -0.525931  
 C 2.111020 1.967392 -1.513871  
 C 0.791166 2.854282 0.258683  
 C 2.690019 3.220547 -1.719275  
 H 2.405355 1.128631 -2.140082  
 C 1.348468 4.115946 0.076126  
 C 2.304409 4.305267 -0.925249  
 H 3.433503 3.350770 -2.502224  
 H 1.034462 4.926780 0.727434  
 H 2.744241 5.288161 -1.076472  
 H -0.297168 -3.175235 -1.746072  
 Cl 4.986670 -1.525112 1.481310  
 F -0.092741 2.716675 1.278235  
 C -3.067216 -0.218920 0.165004  
 O -4.007566 -0.963646 0.442971  
 O -3.209900 1.138571 0.316203  
 C -4.472271 1.577881 0.823747  
 H -4.659027 1.112228 1.799397  
 H -5.276394 1.254555 0.151019  
 C -4.411530 3.094283 0.932480  
 H -5.360376 3.481973 1.326715  
 H -3.601273 3.403598 1.602014  
 H -4.231413 3.548252 -0.048773  
 O -4.791549 -3.734256 0.197341  
 H -4.751790 -2.794903 0.460181  
 H -4.001683 -3.759847 -0.373007

\*\*\*\*

ELZ An1 2w

C -1.339255 -1.058894 0.232795  
 C -0.521678 -2.108093 0.706443  
 C -0.939602 0.359826 0.394336  
 C 1.747398 -1.072719 1.008944  
 C 1.483873 0.203513 0.384685  
 O 2.851109 -1.551808 1.318265  
 N 0.267901 0.825256 0.386789  
 N 0.623964 -1.831669 1.478015  
 C -0.901935 -3.440695 0.488054  
 C -2.087573 -3.763230 -0.175431  
 H -2.377425 -4.798327 -0.325552

C -2.883067 -2.722988 -0.647750  
 C -2.519656 -1.393458 -0.456714  
 H -3.159067 -0.602864 -0.834099  
 H -0.263243 -4.240094 0.858255  
 C -2.030572 1.382524 0.472833  
 C -3.055162 1.273578 1.432606  
 C -2.083782 2.515917 -0.352339  
 C -4.050106 2.242118 1.574268  
 H -3.050323 0.405897 2.087884  
 C -3.061199 3.499029 -0.233935  
 C -4.052469 3.365478 0.741502  
 H -4.816106 2.123173 2.336898  
 H -3.037449 4.346603 -0.913000  
 H -4.819542 4.129459 0.842701  
 H 1.007864 -2.660246 1.922510  
 Cl -4.385609 -3.098504 -1.509830  
 F -1.176266 2.669652 -1.348272  
 C 2.610534 1.028258 -0.051439  
 O 3.774006 0.668851 -0.247006  
 O 2.252121 2.326273 -0.307383  
 C 3.291863 3.175285 -0.802581  
 H 3.703817 2.751574 -1.726626  
 H 4.110306 3.223005 -0.073580  
 C 2.678080 4.546396 -1.042350  
 H 3.439149 5.235966 -1.430878  
 H 1.858934 4.484025 -1.767209  
 H 2.275481 4.961424 -0.111324  
 O 5.569753 -1.286217 0.682774  
 H 5.254745 -0.487763 0.215527  
 H 4.713119 -1.580901 1.055901  
 O 6.583410 -3.161717 -1.109791  
 H 5.815257 -3.253139 -1.692210  
 H 6.285808 -2.499335 -0.435697

\*\*\*\*

ELZ An2 0w

C -1.212811 -0.704249 0.099082  
 C -0.919369 -1.999483 0.660836  
 C -0.203977 0.368610 0.076171  
 C 1.443391 -1.944820 1.029436  
 C 1.575622 -1.105398 -0.314243  
 O 2.458752 -2.154193 1.703759  
 N 1.070316 0.218765 -0.063364  
 N 0.209411 -2.386157 1.303015  
 C -1.988040 -2.954834 0.639438  
 C -3.240083 -2.676464 0.130963  
 H -4.021836 -3.431291 0.133195  
 C -3.497078 -1.394403 -0.387635  
 C -2.512650 -0.427852 -0.391582  
 H -2.730336 0.558101 -0.790931  
 H -1.770629 -3.930866 1.064426  
 C -0.668292 1.782613 0.290306  
 C -1.424115 2.124673 1.424296  
 C -0.342480 2.828765 -0.579260  
 C -1.811056 3.440523 1.683277  
 H -1.698497 1.330822 2.113756  
 C -0.720495 4.149263 -0.353177  
 C -1.456702 4.458205 0.792253  
 H -2.385662 3.669596 2.577234

H -0.437868 4.909632 -1.075420  
 H -1.754592 5.486791 0.981445  
 Cl -5.107630 -1.027750 -1.045050  
 F 0.341263 2.570965 -1.723645  
 C 3.018339 -1.113176 -0.776858  
 O 3.465735 -1.954705 -1.539006  
 O 3.765630 -0.127562 -0.249229  
 C 5.171445 -0.175221 -0.539319  
 H 5.318647 -0.107649 -1.623916  
 H 5.566960 -1.141519 -0.207293  
 C 5.825027 0.984876 0.193103  
 H 6.906343 0.986234 0.003291  
 H 5.410999 1.942090 -0.143483  
 H 5.659694 0.901145 1.272576  
 H 0.996041 -1.626365 -1.090501

\*\*\*\*

ELZ An2 1w

C -1.232198 -0.597259 -0.139512  
 C -0.820657 -1.934848 0.187599  
 C -0.312174 0.547238 -0.000595  
 C 1.549664 -1.746876 0.461293  
 C 1.556076 -0.683417 -0.702085  
 O 2.618616 -2.005709 1.042586  
 N 0.960149 0.533131 -0.205354  
 N 0.370838 -2.321362 0.724369  
 C -1.806320 -2.959521 0.041137  
 C -3.094634 -2.707552 -0.388061  
 H -3.813352 -3.515575 -0.491751  
 C -3.469035 -1.386215 -0.684780  
 C -2.564743 -0.352225 -0.549356  
 H -2.873103 0.664318 -0.772997  
 H -1.499846 -3.970814 0.293586  
 C -0.879756 1.855224 0.475539  
 C -1.580265 1.930895 1.690884  
 C -0.706950 3.054460 -0.222459  
 C -2.060433 3.143383 2.188177  
 H -1.734180 1.013129 2.252091  
 C -1.181977 4.277214 0.242523  
 C -1.859586 4.321591 1.462530  
 H -2.587561 3.167466 3.138439  
 H -1.017885 5.169064 -0.355073  
 H -2.231550 5.271582 1.838624  
 Cl -5.122199 -1.052759 -1.238672  
 F -0.082833 3.050836 -1.428348  
 C 2.974696 -0.483292 -1.204216  
 O 3.443560 -1.122333 -2.130999  
 O 3.666165 0.439822 -0.516921  
 C 5.058600 0.569234 -0.851393  
 H 5.149289 0.868452 -1.902367  
 H 5.538861 -0.408739 -0.737912  
 C 5.655052 1.605432 0.086101  
 H 6.722968 1.735821 -0.131689  
 H 5.154814 2.573201 -0.032161  
 H 5.547424 1.289031 1.129055  
 H 0.984628 -1.103972 -1.542666  
 O 1.608518 -3.985366 2.883529  
 H 0.839124 -3.722613 2.341474  
 H 2.279317 -3.405466 2.467277

\*\*\*\*

ELZ An2 2w

C -1.267009 -0.550614 -0.265516  
C -0.639155 -1.829875 -0.106977  
C -0.535165 0.704821 -0.005421  
C 1.679648 -1.297191 0.109909  
C 1.464544 -0.120258 -0.905970  
O 2.818618 -1.446487 0.604762  
N 0.712313 0.919919 -0.243947  
N 0.626366 -2.070984 0.357217  
C -1.449502 -2.979576 -0.345305  
C -2.775526 -2.892333 -0.724438  
H -3.360425 -3.789913 -0.903243  
C -3.364113 -1.625342 -0.865877  
C -2.633786 -0.478821 -0.625213  
H -3.107373 0.492806 -0.725183  
H -0.983694 -3.950722 -0.204760  
C -1.282108 1.834241 0.645418  
C -1.955817 1.638271 1.862608  
C -1.312519 3.127368 0.113645  
C -2.603502 2.685138 2.520116  
H -1.954457 0.641701 2.295828  
C -1.958110 4.188823 0.740698  
C -2.603843 3.965500 1.958319  
H -3.104658 2.501246 3.466831  
H -1.948378 5.166244 0.267486  
H -3.107984 4.787938 2.459968  
Cl -5.064760 -1.504645 -1.355866  
F -0.726425 3.379974 -1.084588  
C 2.808386 0.361951 -1.425849  
O 3.326882 -0.093612 -2.431057  
O 3.373171 1.312548 -0.665809  
C 4.704082 1.714663 -1.035535  
H 4.682939 2.132909 -2.048781  
H 5.346924 0.827890 -1.051658  
C 5.170733 2.734261 -0.010628  
H 6.187150 3.069530 -0.253880  
H 4.509351 3.607833 0.000906  
H 5.178563 2.296699 0.993283  
H 0.923096 -0.523106 -1.774828  
O 3.783281 -3.522945 2.111558  
H 4.251368 -4.004013 1.413484  
H 3.403883 -2.733083 1.641028  
O 1.052335 -4.534064 1.998356  
H 1.990175 -4.381830 2.231511  
H 0.843778 -3.735164 1.463751

\*\*\*\*

ELZ TS2 0w

C -0.539145 -0.743298 -0.359007  
C 0.081687 -1.776437 -1.090994  
C -0.236015 0.723749 -0.487310  
C 1.962607 -0.552314 -2.010782  
C 2.075652 0.507143 -0.988224  
O 2.828463 -0.328323 -2.930526  
N 0.926217 1.255156 -0.657684  
N 1.030048 -1.491340 -2.113096

C -0.249540 -3.117091 -0.875569  
C -1.193781 -3.474460 0.081926  
H -1.448978 -4.515296 0.249232  
C -1.793327 -2.463530 0.832682  
C -1.477335 -1.126427 0.617444  
H -1.968112 -0.363432 1.210966  
H 0.246904 -3.888562 -1.458586  
C -1.351116 1.689002 -0.230034  
C -1.140755 2.811373 0.590906  
C -2.612176 1.571091 -0.822679  
C -2.152899 3.741654 0.820136  
H -0.159465 2.934919 1.038472  
C -3.638825 2.484787 -0.618211  
C -3.405274 3.578424 0.217136  
H -1.965823 4.594281 1.466820  
H -4.590973 2.334757 -1.117451  
H -4.197715 4.301443 0.389898  
H 1.013182 -2.049365 -2.962095  
Cl -2.969313 -2.883410 2.065608  
H 2.979686 0.709162 -2.241113  
F -2.853185 0.526650 -1.665791  
C 3.150469 0.329579 0.005570  
O 3.120562 1.292827 0.957993  
O 3.988258 -0.562841 -0.033651  
C 4.169786 1.258278 1.956060  
H 4.284960 2.303799 2.254555  
H 5.093831 0.909040 1.488808  
C 3.782983 0.383474 3.140108  
H 3.677764 -0.661897 2.834019  
H 4.562549 0.438554 3.910281  
H 2.839095 0.720707 3.582948

\*\*\*\*

ELZ TS2 1w

C 1.310100 -0.788707 -0.216919  
C 0.714602 -1.989366 -0.651604  
C 0.583893 0.514837 -0.185826  
C -1.743086 -1.527095 -0.454563  
C -1.765628 -0.141714 -0.010327  
O -2.720011 -2.316920 -0.272301  
N -0.676340 0.723036 -0.111761  
N -0.634425 -2.085853 -1.086876  
C 1.468200 -3.170999 -0.681118  
C 2.802832 -3.195921 -0.282403  
H 3.373506 -4.117896 -0.320988  
C 3.383137 -2.016341 0.176049  
C 2.650787 -0.833911 0.206947  
H 3.125018 0.075115 0.557642  
H 1.003017 -4.091545 -1.027007  
C 1.423762 1.762564 -0.232340  
C 2.235120 2.057289 -1.339996  
C 1.385015 2.713364 0.791422  
C 2.953148 3.251185 -1.421542  
H 2.287425 1.338071 -2.153709  
C 2.093586 3.908545 0.742019  
C 2.880952 4.179794 -0.378532  
H 3.562697 3.457278 -2.296960  
H 2.021783 4.602382 1.573934  
H 3.437191 5.111706 -0.432507

H -0.875344 -3.042776 -1.331460  
H -2.331601 -0.693539 1.492232  
Cl 5.056735 -2.017058 0.714137  
O -3.043888 -1.377304 1.989282  
H -3.141165 -1.957239 1.090091  
H -3.862853 -0.840206 1.993144  
F 0.650693 2.462086 1.906744  
C -3.021840 0.632111 -0.358808  
O -3.032851 1.682115 -0.960432  
O -4.190772 0.063566 0.098261  
C -5.415692 0.700047 -0.349354  
H -5.422522 0.698737 -1.443433  
H -5.413542 1.741158 -0.013619  
C -6.580688 -0.086275 0.224148  
H -7.524438 0.355199 -0.116328  
H -6.553234 -1.130845 -0.104530  
H -6.580350 -0.062773 1.320936

\*\*\*\*

ELZ TS2 2w

C 1.356991 -0.758577 -0.342848  
C 0.656653 -1.803845 -0.974167  
C 0.845965 0.640087 -0.350655  
C -1.691464 -0.969107 -1.123438  
C -1.549274 0.248163 -0.359624  
O -2.784139 -1.551697 -1.382792  
N -0.380375 1.013296 -0.361093  
N -0.551201 -1.575259 -1.678693  
C 1.180785 -3.104505 -0.957323  
C 2.388225 -3.390283 -0.322149  
H 2.789626 -4.398401 -0.325454  
C 3.066766 -2.357902 0.323009  
C 2.563968 -1.060691 0.311406  
H 3.115924 -0.267124 0.802548  
H 0.641729 -3.904398 -1.460672  
C 1.862223 1.742760 -0.294575  
C 2.860012 1.866581 -1.275792  
C 1.838214 2.721373 0.705014  
C 3.766645 2.927352 -1.267271  
H 2.907952 1.120186 -2.064925  
C 2.731003 3.786327 0.742806  
C 3.700089 3.891644 -0.256845  
H 4.518229 3.003206 -2.048198  
H 2.658629 4.509753 1.549097  
H 4.401187 4.721737 -0.241582  
H -0.854751 -2.386072 -2.209915  
H -1.808492 -0.517306 1.205637  
Cl 4.581126 -2.696103 1.152809  
O -2.197788 -1.055127 2.029343  
H -3.631041 -1.922736 -0.147834  
O -3.900176 -2.267185 0.792646  
H -3.083493 -1.679600 1.511880  
H -2.575961 -0.387760 2.629921  
H -3.742198 -3.226327 0.796058  
F 0.934066 2.625169 1.714081  
C -2.753747 1.149246 -0.314560  
O -2.761387 2.329345 -0.592268  
O -3.878327 0.511962 0.144025  
C -5.098410 1.290793 0.098778

H -5.249591 1.638962 -0.927795  
H -4.975168 2.174003 0.734000  
C -6.240050 0.407052 0.568452  
H -7.176332 0.977222 0.544834  
H -6.354101 -0.469600 -0.077383  
H -6.079887 0.058003 1.594866

\*\*\*\*

XYZ coordinates for Table S12

CAM 1eq 0w

C 1.293484 -0.477767 -0.066381  
C 1.019051 -1.686152 -0.750768  
C 0.505037 0.761012 -0.320996  
C -1.283512 -1.319066 -1.585545  
C -1.492914 -0.480506 -0.311928  
O -2.161959 -1.552370 -2.395936  
N -0.775581 0.762151 -0.446723  
N 0.018463 -1.774096 -1.753119  
C 1.799361 -2.822103 -0.468466  
C 2.815076 -2.785575 0.479963  
H 3.399283 -3.674636 0.694196  
C 3.062528 -1.595430 1.168071  
C 2.319156 -0.454906 0.896141  
H 2.525368 0.465029 1.432003  
H 1.596508 -3.753013 -0.987402  
C 1.213056 2.070733 -0.419225  
C 2.525286 2.163796 -0.912148  
C 0.540862 3.249623 -0.052299  
C 3.150605 3.406564 -1.037379  
H 3.055727 1.265929 -1.216041  
C 1.169855 4.487797 -0.168488  
C 2.476953 4.571128 -0.661802  
H 4.162886 3.462646 -1.429233  
H 0.641542 5.390133 0.128607  
H 2.965998 5.537745 -0.751984  
H -1.175015 -1.044298 0.574977  
Cl 4.327917 -1.541656 2.383760  
O -2.878720 -0.217972 -0.210526  
C -3.376643 -0.102563 1.060625  
O -2.697504 -0.272067 2.065823  
N -4.703604 0.199872 1.048167  
C -5.398363 0.387711 2.313011  
H -6.246389 -0.306015 2.385297  
H -4.706945 0.200005 3.133810  
H -5.782764 1.414086 2.388844  
C -5.487065 0.410786 -0.163851  
H -6.379515 -0.227859 -0.139541  
H -5.813484 1.458019 -0.230289  
H -4.897073 0.163468 -1.043676  
C 0.266947 -2.600792 -2.941685  
H -0.036668 -3.643405 -2.786309  
H -0.321223 -2.198191 -3.767105  
H 1.329820 -2.559193 -3.187259  
H -0.474700 3.175739 0.322918

\*\*\*\*

CAM 1eq 1w

C -1.372526 -0.465626 -0.113912  
C -0.881310 -1.751463 0.210756  
C -0.730228 0.771084 0.414918  
C 1.410867 -1.276518 0.982639  
C 1.399426 -0.123343 -0.033400  
O 2.392658 -1.565089 1.656800  
N 0.546226 0.927604 0.464826  
N 0.210457 -1.940608 1.102251

C -1.521027 -2.885468 -0.319051  
C -2.613654 -2.765025 -1.169933  
H -3.089752 -3.648697 -1.582119  
C -3.079795 -1.491046 -1.504118  
C -2.475186 -0.355977 -0.980731  
H -2.850506 0.626645 -1.244630  
H -1.145518 -3.873776 -0.074560  
C -1.586995 1.893132 0.895815  
C -2.852723 1.663264 1.460480  
C -1.103413 3.211451 0.826782  
C -3.616761 2.726535 1.947033  
H -3.237190 0.650340 1.537980  
C -1.871505 4.271984 1.303490  
C -3.130798 4.033528 1.865856  
H -4.590032 2.531536 2.389797  
H -1.489539 5.287293 1.234508  
H -3.728410 4.861885 2.237693  
H 1.074616 -0.484380 -1.018253  
Cl -4.445087 -1.325362 -2.594248  
O 2.726109 0.353737 -0.137395  
C 3.064039 0.916598 -1.341531  
O 2.322669 0.908308 -2.315986  
N 4.312025 1.457553 -1.304573  
C 4.856433 2.063779 -2.510817  
H 5.765326 1.533960 -2.826549  
H 4.113593 2.011417 -3.306042  
H 5.115091 3.114122 -2.322307  
C 5.181021 1.445747 -0.133533  
H 6.096471 0.877989 -0.348914  
H 5.465804 2.473399 0.128342  
H 4.670661 0.989727 0.711853  
C 0.150323 -3.035664 2.087305  
H 0.636419 -3.945350 1.720733  
H 0.671914 -2.716583 2.991036  
H -0.896236 -3.234861 2.322297  
H -0.123063 3.385559 0.395184  
O 3.193421 -4.251864 2.251974  
H 4.154306 -4.366485 2.236614  
H 3.035560 -3.297005 2.110581

\*\*\*\*

CAM 1eq 2w

C 1.517730 -0.435242 0.132725  
C 1.159034 -1.802243 0.075202  
C 0.833496 0.587682 -0.707849  
C -1.080659 -1.732597 -0.951340  
C -1.251235 -0.387775 -0.226598  
O -1.970758 -2.253316 -1.613181  
N -0.441212 0.604493 -0.886084  
N 0.172398 -2.288275 -0.826507  
C 1.833001 -2.724524 0.894306  
C 2.830672 -2.315194 1.771522  
H 3.333621 -3.036435 2.407365  
C 3.165328 -0.960295 1.838747  
C 2.525627 -0.032221 1.027974  
H 2.799744 1.015397 1.085593  
H 1.558362 -3.773575 0.855740  
C 1.640407 1.656794 -1.362768  
C 2.965455 1.432392 -1.772564

C 1.052172 2.907960 -1.618151  
C 3.685304 2.435462 -2.425543  
H 3.431791 0.466977 -1.598409  
C 1.775745 3.910910 -2.260410  
C 3.094538 3.678095 -2.666923  
H 4.706116 2.244014 -2.745741  
H 1.312275 4.876998 -2.442796  
H 3.657327 4.461115 -3.168604  
H -0.993803 -0.491247 0.835679  
Cl 4.408131 -0.427590 2.956814  
O -2.618626 -0.035630 -0.334816  
C -3.095676 0.818535 0.617505  
O -2.411259 1.182140 1.574387  
N -4.376420 1.183929 0.372460  
C -5.082573 2.055146 1.306651  
H -5.858713 1.492842 1.842774  
H -4.392655 2.482448 2.031907  
H -5.563661 2.866996 0.748417  
C -5.167850 0.667841 -0.741781  
H -6.013186 0.080008 -0.359749  
H -5.565742 1.505777 -1.327620  
H -4.556396 0.038270 -1.384007  
C 0.408441 -3.562959 -1.529311  
H -0.038562 -4.411226 -1.001543  
H -0.049990 -3.502075 -2.517608  
H 1.484520 -3.707255 -1.635592  
H 0.027037 3.076698 -1.304583  
O -2.487774 -5.074428 -1.554715  
H -3.429516 -5.296207 -1.580163  
H -2.437161 -4.103389 -1.658061  
O -2.783611 2.691323 3.953543  
H -1.944490 3.074050 4.247204  
H -2.566009 2.140504 3.174759

\*\*\*\*

CAM TS2 0w

C 0.556052 -0.364513 0.433330  
C -0.401854 -0.413415 1.473419  
C 1.128151 0.906148 -0.136511  
C -1.186024 1.814273 1.286099  
C -0.989218 1.999664 -0.200216  
O -1.562803 2.956525 1.753891  
N 0.453679 1.958029 -0.456112  
N -0.907671 0.778453 2.069630  
C -0.861756 -1.648127 1.949417  
C -0.409252 -2.844312 1.401238  
H -0.781382 -3.795142 1.768094  
C 0.515829 -2.798218 0.358685  
C 0.998290 -1.582525 -0.111688  
H 1.727607 -1.570538 -0.913878  
H -1.603735 -1.677324 2.740090  
O -1.579330 0.957974 -1.035133  
C 2.602188 0.943680 -0.392882  
C 3.098110 1.738633 -1.441057  
C 3.515120 0.253164 0.422038  
C 4.469515 1.830738 -1.672823  
H 2.390875 2.281228 -2.059717  
C 4.889972 0.358556 0.198253  
C 5.371118 1.142529 -0.853071

H 4.836939 2.441161 -2.493883  
H 5.582954 -0.172835 0.845587  
H 6.440568 1.217199 -1.033257  
Cl 1.086389 -4.294728 -0.362659  
H -1.595211 3.321462 0.682716  
H 3.154808 -0.357101 1.245367  
C -1.262937 0.809098 3.498919  
H -1.192886 1.839328 3.847549  
H -2.287839 0.452297 3.647351  
H -0.563058 0.182276 4.055491  
C -2.878331 0.671799 -0.805650  
N -3.492841 0.097750 -1.882879  
C -4.828219 -0.457292 -1.723874  
H -5.479939 -0.096317 -2.529222  
H -4.804039 -1.556517 -1.764203  
H -5.233589 -0.141024 -0.763282  
C -2.813789 -0.181002 -3.140976  
H -2.524162 -1.240059 -3.213010  
H -3.491675 0.047715 -3.972138  
H -1.921893 0.436752 -3.229253  
O -3.429483 0.896116 0.273045

\*\*\*\*

CAM TS2 1w

C 1.563113 -0.355796 -0.072880  
C 1.181773 -1.575247 -0.671300  
C 0.618011 0.788225 0.070750  
C -1.208724 -1.644520 -0.323791  
C -1.321832 -0.513266 0.575278  
O -2.028515 -2.617526 -0.226972  
N -0.622107 0.658250 0.391697  
N -0.134368 -1.763303 -1.208025  
C 2.111620 -2.625521 -0.745077  
C 3.402820 -2.490632 -0.236521  
H 4.112489 -3.307984 -0.313939  
C 3.762484 -1.294870 0.380002  
C 2.858654 -0.241219 0.461035  
H 3.156976 0.687460 0.934301  
H 1.834244 -3.564830 -1.209099  
O -2.707193 -0.223162 0.862916  
C 1.136732 2.180501 -0.080532  
C 2.171983 2.488299 -0.980296  
C 0.548784 3.230447 0.647523  
C 2.606961 3.805389 -1.146809  
H 2.628903 1.697999 -1.569429  
C 0.989827 4.542965 0.488434  
C 2.021903 4.837776 -0.409828  
H 3.401763 4.023031 -1.856048  
H 0.528127 5.339595 1.066937  
H 2.364315 5.861992 -0.534564  
H -1.426896 -1.533616 1.861039  
Cl 5.377438 -1.110344 1.052298  
O -2.011224 -2.436238 2.195429  
H -2.249328 -2.673523 1.113145  
H -0.260889 2.997923 1.331954  
C -0.314317 -2.783556 -2.247268  
H -0.275509 -3.810949 -1.862862  
H -1.290322 -2.628705 -2.708998  
H 0.464461 -2.640230 -2.999976

C -3.466252 0.157762 -0.221620  
N -4.682621 0.641933 0.159228  
C -5.663081 0.970986 -0.864939  
H -5.193040 0.901226 -1.845306  
H -6.516369 0.278934 -0.821922  
H -6.036185 1.991700 -0.711869  
C -5.136970 0.715515 1.541223  
H -5.618847 1.686352 1.712011  
H -5.869812 -0.075733 1.757737  
H -4.293734 0.612954 2.220960  
O -3.078248 0.054305 -1.375920  
H -1.382619 -3.104379 2.522630

\*\*\*\*

CAM TS2 2w

C -1.528257 -0.375093 0.285476  
C -1.131308 -1.574471 0.917709  
C -0.802896 0.897508 0.523389  
C 1.175225 -1.261858 1.472500  
C 1.340645 -0.091384 0.721949  
O 2.111468 -2.066406 1.807614  
N 0.499259 0.951514 0.603993  
N -0.146872 -1.515033 1.953685  
C -1.739566 -2.788691 0.554201  
C -2.756529 -2.831064 -0.400554  
H -3.243075 -3.768093 -0.651612  
C -3.142062 -1.642853 -1.021793  
C -2.538828 -0.433140 -0.694869  
H -2.848421 0.475444 -1.199165  
H -1.445031 -3.707971 1.050224  
O 2.707741 0.259674 0.487129  
C -1.536205 2.190008 0.488024  
C -2.866984 2.288857 0.934933  
C -0.895994 3.364752 0.047919  
C -3.536446 3.514862 0.934948  
H -3.377423 1.403265 1.303546  
C -1.566173 4.586146 0.042714  
C -2.892030 4.669796 0.485417  
H -4.562073 3.565946 1.292638  
H -1.054411 5.478338 -0.310991  
H -3.413199 5.623817 0.482249  
H 0.674524 -2.134173 -1.313939  
Cl -4.413480 -1.675665 -2.240166  
O 1.535071 -2.166990 -1.777271  
H 2.854857 -2.633840 0.692018  
O 3.183632 -3.059858 -0.218324  
H 2.285565 -2.676622 -1.083964  
H 1.871331 -1.168126 -1.809957  
H 3.232084 -4.020907 -0.097361  
H 0.134264 3.299804 -0.287096  
C -0.235762 -2.500333 3.029822  
H 0.057859 -3.516577 2.729906  
H 0.427045 -2.192850 3.841117  
H -1.266295 -2.512839 3.395964  
C 3.068202 0.589876 -0.761754  
N 4.126192 1.424431 -0.814496  
C 4.746158 2.006951 0.373382  
H 4.091935 1.886546 1.234112  
H 5.709173 1.522852 0.581972

H 4.921178 3.074109 0.195375  
C 4.753988 1.735577 -2.093825  
H 4.702747 2.814880 -2.282658  
H 5.808627 1.432895 -2.075504  
H 4.235962 1.206156 -2.891702  
O 2.510940 0.150477 -1.793168

\*\*\*\*

XYZ coordinates for Table S13

CIN 1eq 0w	H -3.243033 -3.711985 0.572631	C -3.740333 3.591217 1.047581
	C -3.205254 -1.789530 -0.413251	C -3.529110 4.587377 0.093623
	C -2.558833 -0.570618 -0.536270	H -2.294575 5.251566 -1.550366
	H -2.941946 0.181393 -1.216896	H -4.542103 3.677488 1.773821
	H -1.210156 -3.253377 1.906107	H -4.186085 5.452577 0.068951
C 1.376207 -0.495235 -0.389426	O 2.702164 0.695448 -0.006862	H 0.355572 -2.062006 2.134097
C 1.322308 -1.550728 -1.327347	C -1.645506 2.242629 -0.152182	H 1.088021 -0.280597 -0.799481
C 0.439356 0.656158 -0.452110	C -1.350654 3.055967 -1.259698	Br -4.836337 -1.821865 -1.895737
C -0.969799 -1.284125 -2.331293	C -2.729504 2.614834 0.660638	Cl -3.176907 1.289159 2.351651
C -1.413805 -0.707385 -0.977581	C -2.121150 4.175817 -1.566434	C 3.597306 0.179117 -0.436461
O -1.699842 -1.477540 -3.282083	H -0.498953 2.788809 -1.877775	C 4.894410 0.949065 -0.510208
N -0.808991 0.577773 -0.744426	C -3.504829 3.738251 0.368039	H 4.783708 1.745260 -1.255789
N 0.381228 -1.584479 -2.372275	C -3.204983 4.513865 -0.752464	H 5.032574 1.466209 0.446295
C 2.289277 -2.568665 -1.276451	H -1.874858 4.781765 -2.433714	C 6.087669 0.054311 -0.834901
C 3.284718 -2.563590 -0.308114	H -4.327660 4.003202 1.024084	H 6.251560 -0.693962 -0.051289
H 4.023350 -3.357700 -0.280054	H -3.814030 5.384851 -0.978735	H 5.911538 -0.519909 -1.752977
C 3.318695 -1.530649 0.633120	H 0.222082 -1.614140 2.808203	C 7.362273 0.845205 -1.020660
C 2.383861 -0.507737 0.592330	H 1.185190 -0.635316 -0.469322	O 3.474796 -1.018117 -0.654308
H 2.431093 0.300512 1.313470	Br -4.756252 -2.146163 -1.458370	O 7.458566 2.054316 -1.045574
H 2.251805 -3.374669 -2.005123	Cl -3.112155 1.723780 2.129704	O 8.434005 0.026781 -1.176596
O -2.826351 -0.554051 -1.033932	C 3.693907 -0.184391 -0.228960	H 9.215950 0.596976 -1.303525
C 0.945713 2.015994 -0.079439	C 5.015896 0.525984 -0.402012	O 3.116418 -3.555888 0.710127
C 0.276477 2.718076 0.937301	H 4.949808 1.163799 -1.291868	H 3.160886 -4.162051 -0.043810
C 2.041577 2.642252 -0.695347	H 5.145627 1.214713 0.440021	H 3.259859 -2.662163 0.338479
C 0.699592 3.981587 1.345923	C 6.187852 -0.445687 -0.514205	O 1.036823 -3.773687 2.552705
H -0.582942 2.246488 1.404267	H 6.315845 -1.025500 0.406682	H 1.812731 -3.755033 1.942111
C 2.469774 3.910767 -0.301090	H 6.008181 -1.187792 -1.301973	H 1.409449 -3.845666 3.444195
C 1.800966 4.577381 0.726532	C 7.487677 0.258297 -0.828333	
H 0.169865 4.498877 2.140799	O 3.531841 -1.391666 -0.309060	****
H 3.312628 4.370635 -0.806882	O 7.617142 1.428954 -1.120011	CIN An1 0w
H 2.139473 5.563213 1.033571	O 8.541556 -0.594902 -0.762307	
H 0.648157 -2.080530 -3.216637	H 9.340925 -0.083166 -0.990002	C -1.428482 -0.436606 0.456040
H -1.164095 -1.419226 -0.178035	O 1.687677 -3.468595 0.521092	C -1.022215 -1.578229 1.189147
Br 4.664206 -1.527859 1.978585	H 2.000231 -4.339778 0.236176	C -0.650955 0.813007 0.453997
Cl 2.880900 1.878917 -2.042077	H 2.385880 -2.841489 0.248924	C 1.373108 -1.184259 1.766347
C -3.485648 -0.569353 0.151780		C 1.538951 -0.066627 0.875631
C -4.954081 -0.276931 -0.057664	****	O 2.297587 -1.805434 2.310137
H -5.047022 0.784870 -0.318780	CIN 1eq 2w	N 0.674336 0.841130 0.509843
H -5.303296 -0.824076 -0.939694		N 0.036795 -1.500162 2.134469
C -5.789453 -0.600621 1.178950	C -1.481870 -0.209730 0.016874	C -1.728389 -2.780019 1.069696
H -5.797081 -1.675699 1.390973	C -0.919815 -1.335037 0.667739	C -2.872539 -2.885885 0.273111
H -5.355716 -0.132132 2.071337	C -0.912075 1.154480 0.149455	H -3.425923 -3.817132 0.213539
C -7.216760 -0.120845 1.052525	C 1.319266 -0.485479 1.341641	C -3.270170 -1.760464 -0.440363
O -2.948976 -0.781626 1.220212	C 1.292200 0.373429 0.060538	C -2.562079 -0.567391 -0.374483
O -7.651547 0.620700 0.196331	O 2.264507 -0.507510 2.110989	H -2.887456 0.283044 -0.962741
O -7.995434 -0.611602 2.051200	N 0.343820 1.434163 0.183577	H -1.392404 -3.646674 1.636376
H -8.891035 -0.245277 1.923086	N 0.195922 -1.256072 1.512041	O 2.906097 0.347126 0.760844
****	C -1.557124 -2.585911 0.555653	C -1.271116 2.094663 0.043205
CIN 1eq 1w	C -2.712186 -2.734868 -0.198017	C -0.605044 2.918201 -0.898460
	H -3.190406 -3.705891 -0.275559	C -2.479820 2.620387 0.553302
	C -3.253742 -1.624177 -0.853929	C -1.110811 4.141944 -1.319827
C -1.410687 -0.286950 0.227770	C -2.655482 -0.380384 -0.743800	H 0.340011 2.551848 -1.286856
C -0.924219 -1.269848 1.119881	H -3.096073 0.478530 -1.237567	C -3.008138 3.843992 0.132500
C -0.776032 1.049160 0.102981	H -1.129595 -3.439118 1.075187	C -2.329405 4.612779 -0.812206
C 1.356788 -0.415354 1.676005	O 2.572745 0.988495 -0.126731	H -0.560699 4.727238 -2.053931
C 1.395978 0.169888 0.248619	C -1.843997 2.328184 0.168755	H -3.940536 4.192977 0.566705
O 2.282281 -0.346942 2.461676	C -1.638384 3.358432 -0.764486	H -2.741685 5.565373 -1.136438
N 0.490858 1.270788 0.126808	C -2.903607 2.474194 1.079957	H 0.073134 -2.307132 2.749687
N 0.165314 -1.036607 1.975488	C -2.471900 4.474216 -0.812564	Br -4.817097 -1.871398 -1.575668
C -1.599768 -2.495616 1.232633	H -0.805872 3.263762 -1.455033	Cl -3.368389 1.785341 1.838112
C -2.733708 -2.758734 0.477768		

C 3.689577 -0.283874 -0.123946  
C 5.119517 0.228166 -0.012109  
H 5.145261 1.260319 -0.382422  
H 5.391802 0.281593 1.047079  
C 6.092421 -0.650010 -0.794361  
H 6.148726 -1.658085 -0.368545  
H 5.730086 -0.796875 -1.820421  
C 7.485486 -0.081666 -0.876827  
O 3.332318 -1.126630 -0.924643  
O 7.836362 1.046879 -0.595258  
O 8.378007 -1.001419 -1.348477  
H 9.240419 -0.547970 -1.394910

\*\*\*\*

CIN An1 1w

C -1.476782 -0.364512 0.267256  
C -1.039973 -1.611288 0.771746  
C -0.724829 0.884880 0.494084  
C 1.346540 -1.268202 1.380827  
C 1.483592 -0.009032 0.722116  
O 2.315135 -1.953728 1.786091  
N 0.593593 0.939923 0.546682  
N 0.037761 -1.697138 1.695870  
C -1.731465 -2.783586 0.447768  
C -2.884365 -2.759744 -0.342412  
H -3.427258 -3.673368 -0.560368  
C -3.307484 -1.532229 -0.838950  
C -2.616713 -0.358609 -0.562240  
H -2.963296 0.580064 -0.979140  
H -1.378301 -3.730189 0.851485  
O 2.837704 0.452186 0.670510  
C -1.389408 2.204215 0.347376  
C -0.777960 3.202196 -0.449049  
C -2.589384 2.587413 0.985528  
C -1.328353 4.466976 -0.621528  
H 0.159281 2.940186 -0.929952  
C -3.160906 3.851629 0.816057  
C -2.535998 4.799272 0.006229  
H -0.821754 5.193104 -1.253886  
H -4.083886 4.088044 1.337397  
H -2.982439 5.782313 -0.123435  
H 0.086019 -2.605380 2.151658  
Br -4.864325 -1.462971 -1.962130  
Cl -3.407406 1.499558 2.116426  
C 3.626643 0.009767 -0.318299  
C 5.039242 0.547811 -0.135783  
H 5.020177 1.630124 -0.312807  
H 5.330803 0.420566 0.911959  
C 6.027918 -0.135722 -1.076407  
H 6.126693 -1.201893 -0.843528  
H 5.654660 -0.105468 -2.108539  
C 7.399064 0.489705 -1.065983  
O 3.284086 -0.698360 -1.245789  
O 7.715525 1.556331 -0.578281  
O 8.313174 -0.289889 -1.714679  
H 9.159165 0.194776 -1.683429  
O 1.540199 -4.471079 2.520977  
H 1.724712 -5.002306 1.732766  
H 1.950365 -3.587902 2.326599

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CIN An1 2w

C -1.560338 -0.442857 0.241014  
C -1.180428 -1.686216 0.796367  
C -0.768365 0.788279 0.431508  
C 1.212306 -1.415490 1.395881  
C 1.401051 -0.184206 0.706225  
O 2.155131 -2.131648 1.809733  
N 0.548847 0.809481 0.509530  
N -0.112500 -1.783031 1.727755  
C -1.922051 -2.838517 0.511297  
C -3.069198 -2.792653 -0.284971  
H -3.650646 -3.689415 -0.471580  
C -3.439562 -1.567352 -0.827336  
C -2.698404 -0.416202 -0.589714  
H -3.004490 0.521705 -1.038517  
H -1.612129 -3.784096 0.950913  
O 2.770582 0.218988 0.635325  
C -1.406648 2.116317 0.228036  
C -0.828379 3.035375 -0.675806  
C -2.561845 2.562152 0.903968  
C -1.364125 4.299290 -0.901953  
H 0.067743 2.722063 -1.202930  
C -3.119455 3.823116 0.680346  
C -2.523242 4.698355 -0.227654  
H -0.880073 4.970520 -1.607349  
H -4.006378 4.115857 1.234394  
H -2.956281 5.681366 -0.396320  
H -0.098286 -2.679244 2.209655  
Br -4.992531 -1.468116 -1.951632  
Cl -3.335137 1.557635 2.135712  
C 3.527784 -0.276086 -0.361612  
C 4.972116 0.162637 -0.182538  
H 4.997559 1.246758 -0.023987  
H 5.348493 -0.285232 0.744601  
C 5.836691 -0.241647 -1.373144  
H 5.760383 -1.320724 -1.556420  
H 5.481955 0.225919 -2.299259  
C 7.294468 0.099546 -1.197273  
O 3.132021 -0.975148 -1.272088  
O 7.826944 0.552491 -0.204442  
O 8.012844 -0.172507 -2.325861  
H 8.938303 0.062898 -2.126703  
O 1.244040 -4.547850 2.700234  
H 1.433390 -5.161238 1.975477  
H 1.711436 -3.708923 2.447795  
O 2.290415 3.213063 1.102971  
H 2.979064 2.632299 1.460865  
H 1.601376 2.566442 0.835561

\*\*\*\*

CIN An2 0w

C -1.377031 -0.549102 0.372881  
C -1.174294 -1.682426 1.243509  
C -0.473040 0.605739 0.393808  
C 0.950663 -1.256985 2.268540  
C 1.421864 -0.678161 0.890904

O 1.706504 -1.208738 3.243263  
N 0.793727 0.577027 0.649582  
N -0.269992 -1.814148 2.241839  
C -2.126676 -2.747962 1.120076  
C -3.195477 -2.706904 0.250975  
H -3.895420 -3.536011 0.196837  
C -3.377464 -1.570727 -0.558851  
C -2.495994 -0.514072 -0.493946  
H -2.650207 0.355585 -1.124381  
H -1.981201 -3.602226 1.775494  
O 2.852081 -0.463626 0.949819  
C -0.998350 1.965286 0.017384  
C -0.403012 2.630971 -1.067806  
C -2.028275 2.636775 0.695245  
C -0.827485 3.893786 -1.479365  
H 0.409835 2.127317 -1.582735  
C -2.462076 3.905003 0.299006  
C -1.864969 4.532460 -0.794868  
H -0.349147 4.376753 -2.327957  
H -3.256121 4.393031 0.855826  
H -2.207732 5.517632 -1.102538  
H 1.221618 -1.397679 0.087560  
Br -4.872704 -1.503154 -1.763984  
Cl -2.784649 1.929785 2.118826  
C 3.540008 -0.472136 -0.191648  
C 5.001870 -0.133424 0.065693  
H 5.086666 0.960248 0.092329  
H 5.283443 -0.486542 1.062237  
C 5.910851 -0.704802 -1.021381  
H 5.963714 -1.797963 -0.969965  
H 5.488983 -0.478646 -2.010169  
C 7.311906 -0.149299 -0.988592  
O 3.086052 -0.705271 -1.300679  
O 7.679332 0.876180 -0.452029  
O 8.182916 -0.936163 -1.685229  
H 9.049919 -0.490760 -1.643646

\*\*\*\*

CIN An2 1w

C -1.432923 -0.507398 -0.123186  
C -1.212863 -1.928777 -0.058902  
C -0.530606 0.440182 0.543959  
C 0.937553 -2.134382 0.960143  
C 1.372460 -0.869185 0.161013  
O 1.736916 -2.647874 1.763798  
N 0.741408 0.287680 0.708497  
N -0.280884 -2.590026 0.675922  
C -2.161653 -2.749589 -0.746891  
C -3.243452 -2.233907 -1.429593  
H -3.941457 -2.893561 -1.937055  
C -3.441442 -0.842035 -1.449077  
C -2.565085 0.002430 -0.802460  
H -2.733999 1.074090 -0.821947  
H -2.004011 -3.822968 -0.691319  
O 2.803323 -0.709555 0.285786  
C -1.070446 1.756958 1.032253  
C -0.507520 2.937784 0.519135  
C -2.085728 1.891391 1.992689  
C -0.951129 4.197448 0.920291

H 0.294283 2.840033 -0.206894  
C -2.537460 3.146640 2.409235  
C -1.973819 4.302040 1.866865  
H -0.499154 5.091434 0.497838  
H -3.318967 3.207959 3.160319  
H -2.330942 5.276865 2.190519  
H 1.138071 -0.995740 -0.903301  
Br -4.953881 -0.119406 -2.386295  
Cl -2.796490 0.476199 2.759199  
C 3.436921 -0.001970 -0.652561  
C 4.910016 0.147967 -0.302359  
H 4.995742 0.975718 0.412859  
H 5.247025 -0.747903 0.227981  
C 5.757330 0.431027 -1.541548  
H 5.811240 -0.441802 -2.201647  
H 5.283729 1.220398 -2.140707  
C 7.159308 0.883587 -1.220692  
O 2.925220 0.474569 -1.652301  
O 7.559892 1.326247 -0.163425  
O 7.984137 0.770918 -2.301689  
H 8.854118 1.112842 -2.022255  
O 1.712514 -4.770494 3.564765  
H 1.534942 -4.105615 2.854880  
H 2.439101 -4.363269 4.058380

\*\*\*\*

CIN An2 2w

C -1.393613 -0.237006 -0.200430  
C -1.214808 -1.658037 -0.298767  
C -0.487312 0.602396 0.597966  
C 0.931274 -2.031277 0.695653  
C 1.390542 -0.686944 0.066698  
O 1.725222 -2.664729 1.419193  
N 0.777918 0.404749 0.755850  
N -0.300545 -2.423448 0.371681  
C -2.171536 -2.371816 -1.081275  
C -3.224586 -1.748564 -1.720604  
H -3.932398 -2.328375 -2.305420  
C -3.378385 -0.358447 -1.594749  
C -2.492247 0.381756 -0.841686  
H -2.628997 1.453605 -0.743823  
H -2.055915 -3.449929 -1.144613  
O 2.821471 -0.573470 0.211748  
C -1.015050 1.852913 1.245820  
C -0.411866 3.077792 0.913586  
C -2.056257 1.879446 2.187647  
C -0.841180 4.281720 1.470693  
H 0.409135 3.059622 0.202865  
C -2.493254 3.077636 2.759099  
C -1.889378 4.281533 2.394784  
H -0.358172 5.213385 1.186987  
H -3.295287 3.056061 3.490432  
H -2.235332 5.211747 2.839160  
H 1.155474 -0.673534 -1.005107  
Br -4.846707 0.511978 -2.470893  
Cl -2.817969 0.391852 2.734632  
C 3.466950 0.248813 -0.621656  
C 4.941389 0.326665 -0.257332  
H 5.040630 1.050560 0.561306

H 5.263791 -0.636606 0.149470  
C 5.793712 0.757723 -1.449541  
H 5.828324 -0.018257 -2.222367  
H 5.338223 1.631397 -1.934762  
C 7.205676 1.130703 -1.073684  
O 2.960067 0.865294 -1.543626  
O 7.617710 1.402170 0.035582  
O 8.023774 1.164528 -2.164567  
H 8.901853 1.443808 -1.843816  
O 1.490112 -5.192830 2.459909  
H 1.510671 -4.244528 2.162280  
H 2.219228 -5.603411 1.972696  
O -0.886392 -5.322575 0.773377  
H -0.184787 -5.525168 1.424063  
H -0.753962 -4.359325 0.624164

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CIN TS2 0w

C 1.320299 -0.637800 0.314476  
C 1.351485 -1.931969 0.876302  
C 0.162319 0.318960 0.332778  
C -1.016943 -2.243971 1.376551  
C -1.677469 -1.214149 0.541662  
O -1.940440 -2.837308 2.060405  
N -1.096535 0.046540 0.317581  
N 0.265961 -2.458338 1.628972  
C 2.486971 -2.738769 0.770792  
C 3.622333 -2.295096 0.099633  
H 4.500502 -2.926941 0.024917  
C 3.599148 -1.027653 -0.477162  
C 2.474544 -0.217623 -0.373652  
H 2.488756 0.765118 -0.827970  
H 2.479086 -3.730423 1.216356  
O -2.126379 -1.805094 -0.694145  
C 0.485927 1.780048 0.181441  
C -0.011811 2.477909 -0.931266  
C 1.226653 2.505395 1.126537  
C 0.241560 3.836899 -1.108315  
H -0.603484 1.929414 -1.658280  
C 1.481702 3.868720 0.968076  
C 0.992440 4.533264 -0.157020  
H -0.148378 4.350420 -1.982576  
H 2.049697 4.398959 1.725764  
H 1.193570 5.593676 -0.282286  
H 0.488123 -3.071564 2.409222  
H -2.608252 -1.932375 1.626075  
C -3.350625 -1.494843 -1.218536  
O -3.651438 -1.990230 -2.280125  
C -4.243956 -0.547097 -0.436117  
H -4.550766 -1.041205 0.493052  
H -3.663238 0.330995 -0.134330  
C -5.476329 -0.146712 -1.261769  
H -5.182940 0.383321 -2.170071  
H -6.020237 -1.048149 -1.566555  
C -6.421376 0.747772 -0.493625  
O -6.781003 1.857115 -0.827270  
O -6.862206 0.162832 0.654695  
H -7.469386 0.795867 1.082393  
Br 5.121956 -0.391243 -1.419516

Cl 1.823707 1.720044 2.588722

\*\*\*\*

CIN TS2 1w

C -1.589839 -0.558146 0.004777  
C -1.357710 -1.799253 0.629936  
C -0.498652 0.387137 -0.366519  
C 1.064076 -2.232795 0.171284  
C 1.305329 -1.157771 -0.765444  
O 1.833297 -3.252862 0.196976  
N 0.698250 0.075145 -0.709501  
N -0.065678 -2.293459 0.952009  
C -2.442030 -2.611367 0.985870  
C -3.754924 -2.226011 0.724635  
H -4.580859 -2.865822 1.016704  
C -3.982334 -1.014138 0.079432  
C -2.917427 -0.194532 -0.275722  
H -3.111276 0.753362 -0.763996  
H -2.257614 -3.562169 1.481084  
O 2.739902 -0.976460 -0.992992  
C -0.828052 1.848936 -0.455708  
C -1.318425 2.606025 0.621483  
C -0.602102 2.523316 -1.668073  
C -1.591684 3.969549 0.494307  
C -0.873620 3.882868 -1.811610  
C -1.374957 4.607886 -0.727277  
H -1.959429 4.521821 1.353247  
H -0.694737 4.373510 -2.764509  
H -1.591578 5.668344 -0.824398  
H -0.091759 -3.184652 1.439056  
H 1.407880 -2.282965 -1.985940  
O 1.940493 -3.229656 -2.234074  
H 2.104765 -3.425691 -1.141035  
H 2.790814 -2.941875 -2.612900  
Br -5.763386 -0.472609 -0.323967  
C 3.463674 -0.501929 0.063403  
O 3.025697 -0.387518 1.183965  
C 4.867005 -0.131497 -0.374328  
H 5.262887 -0.931079 -1.011998  
H 4.788059 0.759590 -1.009111  
C 5.790902 0.132938 0.824228  
H 5.354099 0.921275 1.447240  
H -0.204007 1.952342 -2.501837  
Cl -1.549306 1.873386 2.206519  
H 5.894243 -0.762577 1.440381  
C 7.175763 0.558893 0.395059  
O 8.205947 -0.041201 0.617963  
O 7.157841 1.731177 -0.296678  
H 8.081846 1.940055 -0.531218

\*\*\*\*

CIN TS2 2w

C -1.684481 -0.423506 0.179843  
C -1.432732 -1.595736 0.918037  
C -0.619585 0.567842 -0.135348  
C 1.041303 -1.887456 0.748997  
C 1.234608 -0.941718 -0.322259  
O 1.894476 -2.769599 1.067623



N 0.612312 0.287559 -0.375092  
N -0.154290 -1.908698 1.446725  
C -2.482585 -2.479581 1.198802  
C -3.778302 -2.228553 0.752338  
H -4.581606 -2.918942 0.986665  
C -4.018965 -1.083084 -0.001803  
C -2.989491 -0.193240 -0.285261  
H -3.195484 0.703565 -0.858604  
H -2.285011 -3.375505 1.783384  
O 2.639648 -0.811121 -0.662565  
C -1.007353 2.002691 -0.329859  
C -1.679024 2.772593 0.635301  
C -0.655925 2.643951 -1.531117  
C -2.004875 4.111706 0.408805  
C -0.976354 3.978094 -1.773090  
C -1.658814 4.714362 -0.800716  
H -2.514697 4.674104 1.184616  
H -0.695792 4.440682 -2.715543  
H -1.916315 5.755683 -0.974801  
H -0.159915 -2.689497 2.095544  
H 1.060627 -1.956791 -1.641518  
O 1.339553 -2.700950 -2.375132  
H 2.661464 -3.308778 -0.029705  
O 2.994143 -3.754633 -0.942521  
H 2.237483 -3.303040 -1.733272  
H 1.734067 -2.210806 -3.117694  
H 2.870513 -4.715499 -0.860757  
H -0.117689 2.065054 -2.275787  
Br -5.774369 -0.731342 -0.655863  
Cl -2.082551 2.095693 2.211168  
C 3.440014 -0.165853 0.237319  
O 3.080264 0.192170 1.333346  
C 4.824675 0.041636 -0.346177  
H 5.166289 -0.905512 -0.780955  
H 4.731980 0.749389 -1.178856  
C 5.815988 0.562986 0.704622  
H 5.933132 -0.154899 1.518910  
H 5.428912 1.494330 1.133323  
C 7.185206 0.827112 0.123757  
O 8.217951 0.285371 0.457713  
O 7.153053 1.775726 -0.853146  
H 8.069617 1.893432 -1.166727

\*\*\*\*

## XYZ coordinates for Table S14

## MCZ 1eq 0w

C -0.606704 -0.554927 0.091986  
 C -1.132913 -1.797814 0.529817  
 C 0.855361 -0.267610 0.107142  
 C 0.900684 -3.279779 0.440256  
 C 1.452786 -2.424410 -0.703725  
 O 1.427988 -4.283843 0.881100  
 N 1.786429 -1.096485 -0.187538  
 N -0.316577 -2.842059 0.966699  
 C -2.530582 -1.977388 0.606257  
 C -3.404067 -0.970628 0.233015  
 H -4.477645 -1.108685 0.280638  
 C -2.874474 0.240820 -0.224480  
 C -1.504490 0.457467 -0.280183  
 H -1.133213 1.422260 -0.604923  
 H -2.922617 -2.929773 0.953638  
 C 1.272944 1.105009 0.550646  
 C 0.958780 1.523678 1.854243  
 C 1.996210 1.989194 -0.265848  
 C 1.373405 2.761701 2.341491  
 H 0.392157 0.853133 2.495574  
 C 2.407820 3.237452 0.207699  
 C 2.102044 3.619660 1.513866  
 H 1.127741 3.054897 3.358156  
 H 2.958311 3.901493 -0.450733  
 H 2.427338 4.590399 1.877790  
 H -0.737822 -3.524155 1.590185  
 H 0.647159 -2.340884 -1.453909  
 Cl 2.365026 1.590183 -1.937403  
 C 2.683426 -3.061901 -1.338784  
 H 3.048508 -2.416171 -2.143221  
 H 3.477506 -3.180774 -0.596992  
 H 2.442897 -4.046832 -1.750893  
 N -3.788333 1.314623 -0.633482  
 O -4.999084 1.100445 -0.537503  
 O -3.294876 2.365436 -1.046045

\*\*\*\*

## MCZ 1eq 1w

C 0.821766 0.586098 0.087202  
 C 1.254463 1.859769 0.540286  
 C -0.613694 0.193319 0.088118  
 C -0.867865 3.206111 0.415906  
 C -1.346618 2.310847 -0.731699  
 O -1.459191 4.182371 0.833514  
 N -1.595797 0.962662 -0.213117  
 N 0.363038 2.842916 0.969798  
 C 2.635671 2.133130 0.636983  
 C 3.580563 1.192521 0.265410  
 H 4.641443 1.403919 0.327331  
 C 3.141750 -0.048120 -0.209899  
 C 1.791481 -0.359100 -0.282785  
 H 1.491807 -1.344314 -0.619850  
 H 2.957260 3.106847 0.997078  
 C -0.933783 -1.206106 0.523941  
 C -0.574652 -1.611689 1.820438

C -1.604591 -2.132492 -0.290332  
 C -0.896635 -2.878842 2.301150  
 H -0.050718 -0.907760 2.461949  
 C -1.918813 -3.410817 0.174862  
 C -1.571456 -3.779980 1.474179  
 H -0.621799 -3.160749 3.313368  
 H -2.429177 -4.107028 -0.482549  
 H -1.824379 -4.773375 1.834045  
 H 0.730323 3.553674 1.595680  
 H -0.525174 2.273027 -1.467265  
 Cl -2.030124 -1.745204 -1.954178  
 C -2.603748 2.867791 -1.390682  
 H -2.907488 2.207600 -2.208995  
 H -3.423367 2.931848 -0.670669  
 H -2.414870 3.867765 -1.792637  
 N 4.132358 -1.051923 -0.619781  
 O 5.323742 -0.754674 -0.509212  
 O 3.716292 -2.129548 -1.047725  
 O -4.449943 0.177909 0.312943  
 H -4.701407 -0.417811 -0.408246  
 H -3.517773 0.416155 0.128849

\*\*\*\*

## MCZ 1eq 2w

C -0.182853 0.911990 -0.159932  
 C -0.106987 2.270972 -0.565859  
 C 1.021757 0.039690 -0.085744  
 C 2.332668 2.781597 -0.212669  
 C 2.373053 1.737856 0.907700  
 O 3.256698 3.502966 -0.530476  
 N 2.180200 0.406044 0.326612  
 N 1.101151 2.894009 -0.868584  
 C -1.295343 3.012959 -0.746271  
 C -2.535255 2.452092 -0.499845  
 H -3.447080 3.023664 -0.625687  
 C -2.595102 1.121805 -0.067304  
 C -1.447022 0.355046 0.083324  
 H -1.536484 -0.683042 0.380394  
 H -1.227569 4.047939 -1.070645  
 C 0.869599 -1.368710 -0.577629  
 C 0.485200 -1.584365 -1.911985  
 C 1.120893 -2.494855 0.222954  
 C 0.383065 -2.869139 -2.440481  
 H 0.283371 -0.723237 -2.543975  
 C 1.006151 -3.787696 -0.291608  
 C 0.644861 -3.973260 -1.625864  
 H 0.099932 -3.007096 -3.479850  
 H 1.196559 -4.637772 0.355296  
 H 0.563170 -4.981216 -2.022797  
 H 1.057781 3.711760 -1.469764  
 H 1.531785 1.967027 1.583692  
 Cl 1.536269 -2.331330 1.925594  
 C 3.686328 1.794742 1.680595  
 H 3.672410 1.041400 2.474208  
 H 4.533413 1.592034 1.020552  
 H 3.824140 2.782372 2.130861  
 N -3.897565 0.519525 0.209328  
 O -4.904456 1.210024 0.038472  
 O -3.921688 -0.653825 0.600176

O 4.628492 -1.273675 -0.143260  
 H 4.633987 -1.958594 0.541622  
 H 3.818904 -0.750361 0.029211  
 O -6.841313 -1.420204 1.068905  
 H -7.229664 -0.568516 0.818592  
 H -5.885676 -1.287408 0.944873

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## MCZ An1 0w

C 0.671764 0.503204 0.189827  
 C 1.234816 1.781572 0.478427  
 C -0.780360 0.247727 0.254332  
 C -0.745285 3.347075 0.312688  
 C -1.750317 2.440550 -0.143807  
 O -0.850047 4.587816 0.318163  
 N -1.741666 1.113725 0.012777  
 N 0.453848 2.836280 0.946085  
 C 2.629216 1.977055 0.391474  
 C 3.495991 0.950054 0.043734  
 H 4.567254 1.102051 -0.004265  
 C 2.944827 -0.297931 -0.257970  
 C 1.561310 -0.512399 -0.198571  
 H 1.180587 -1.497312 -0.436770  
 H 3.031490 2.961063 0.623959  
 C -1.235590 -1.149275 0.503272  
 C -0.754988 -1.843305 1.638297  
 C -2.176833 -1.849285 -0.283481  
 C -1.190866 -3.118002 1.986390  
 H -0.026121 -1.336349 2.265944  
 C -2.635888 -3.124218 0.058919  
 C -2.148738 -3.765976 1.197933  
 H -0.793312 -3.600850 2.876542  
 H -3.360899 -3.614220 -0.584580  
 H -2.506156 -4.759950 1.456401  
 H 1.003529 3.648925 1.209965  
 Cl -2.789135 -1.178054 -1.797934  
 C -3.042765 3.073548 -0.617230  
 H -3.755308 2.279428 -0.860337  
 H -3.488504 3.733588 0.142795  
 H -2.891202 3.694522 -1.511732  
 N 3.825647 -1.382438 -0.639176  
 O 5.051682 -1.168694 -0.673737  
 O 3.327286 -2.484037 -0.916440

\*\*\*\*

## MCZ An1 1w

C 0.225796 0.778205 0.225472  
 C -0.673799 1.828822 0.565101  
 C -0.164456 -0.647135 0.295147  
 C -2.931208 0.714173 0.458636  
 C -2.569131 -0.567042 -0.029276  
 O -4.098504 1.171085 0.512470  
 N -1.360643 -1.141927 0.094078  
 N -1.942208 1.564954 1.078910  
 C -0.255703 3.172936 0.479008  
 C 1.027624 3.516613 0.076841  
 H 1.348780 4.549753 0.025881  
 C 1.903376 2.487595 -0.277045

C 1.506597 1.145383 -0.213647  
H 2.221342 0.380289 -0.488996  
H -0.959865 3.956264 0.751388  
C 0.915072 -1.655724 0.509966  
C 1.761887 -1.532418 1.634278  
C 1.138514 -2.785702 -0.305018  
C 2.739810 -2.471975 1.947900  
H 1.618750 -0.670171 2.280970  
C 2.108331 -3.744537 0.001120  
C 2.912015 -3.595118 1.131557  
H 3.358873 -2.334040 2.831569  
H 2.238204 -4.595006 -0.661762  
H 3.667280 -4.342453 1.362785  
H -2.432091 2.403577 1.376754  
Cl 0.241764 -3.026644 -1.805955  
C -3.700449 -1.458812 -0.498291  
H -3.293453 -2.448177 -0.727510  
H -4.490008 -1.570217 0.260824  
H -4.182629 -1.069242 -1.407324  
N 3.244243 2.821377 -0.714715  
O 3.574845 4.019994 -0.750834  
O 4.009998 1.900447 -1.035245  
O -6.732570 0.734694 -0.387051  
H -6.671358 -0.150984 -0.773253  
H -5.819368 0.911181 -0.063218

\*\*\*\*

MCZ An1 2w

C 0.046234 -0.689299 0.303731  
C 0.787020 -1.875640 0.586239  
C 0.665595 0.654518 0.328535  
C 3.195282 -1.124433 0.310490  
C 3.009904 0.207938 -0.132391  
O 4.277261 -1.758104 0.291853  
N 1.909930 0.956153 0.059368  
N 2.121294 -1.841560 0.960159  
C 0.138773 -3.131475 0.577903  
C -1.211644 -3.256808 0.294355  
H -1.703966 -4.221727 0.297828  
C -1.931771 -2.098926 -0.014636  
C -1.309197 -0.840575 -0.017244  
H -1.907183 0.031536 -0.247605  
H 0.722368 -4.019702 0.809689  
C -0.227098 1.824442 0.590476  
C -0.984631 1.865564 1.781390  
C -0.341085 2.949728 -0.251385  
C -1.779523 2.954024 2.129604  
H -0.921481 1.010809 2.450604  
C -1.126043 4.055777 0.087257  
C -1.847139 4.064598 1.281253  
H -2.337424 2.940190 3.063129  
H -1.178570 4.896794 -0.597847  
H -2.459501 4.925550 1.538296  
H 2.493502 -2.751881 1.214186  
Cl 0.462756 3.002579 -1.821159  
C 4.238017 0.924642 -0.654114  
H 3.976678 1.968323 -0.851991  
H 5.072672 0.900759 0.063200  
H 4.607514 0.481039 -1.590502

N -3.330343 -2.210918 -0.328137  
O -3.870746 -3.329440 -0.308309  
O -3.959673 -1.168706 -0.612342  
O 6.930112 -1.694065 -0.671710  
H 6.993181 -0.800085 -1.037957  
H 6.009044 -1.741802 -0.328262  
O -6.812394 -0.890508 -1.157091  
H -5.914849 -1.232152 -0.969715  
H -6.677651 0.064917 -1.241056

\*\*\*\*

MCZ An2 0w

C 0.590432 0.627184 0.084109  
C 1.054078 1.964798 0.426331  
C -0.845891 0.281295 0.066971  
C -0.992191 3.193051 0.544410  
C -1.542724 2.413845 -0.689980  
O -1.729563 3.964068 1.166911  
N -1.825282 1.058027 -0.236929  
N 0.320588 3.003810 0.834605  
C 2.484760 2.161303 0.422588  
C 3.378749 1.167964 0.124520  
H 4.447469 1.349491 0.125330  
C 2.896230 -0.128991 -0.183737  
C 1.523769 -0.380961 -0.180402  
H 1.186945 -1.387548 -0.401159  
H 2.827967 3.158510 0.682669  
C -1.235072 -1.107595 0.507026  
C -0.985089 -1.489074 1.836167  
C -1.877530 -2.042007 -0.318005  
C -1.377408 -2.731299 2.331759  
H -0.477415 -0.779913 2.484694  
C -2.269385 -3.296223 0.159373  
C -2.024131 -3.639266 1.488817  
H -1.175570 -2.990100 3.368115  
H -2.755935 -3.994462 -0.514628  
H -2.330312 -4.615262 1.857740  
H -0.750868 2.390600 -1.456744  
Cl -2.181638 -1.696885 -2.019828  
C -2.804016 3.042807 -1.271531  
H -3.175069 2.435142 -2.106039  
H -3.580873 3.107601 -0.504746  
H -2.596426 4.056836 -1.633249  
N 3.815142 -1.182570 -0.485647  
O 5.038154 -0.930879 -0.460766  
O 3.372323 -2.315654 -0.761096

\*\*\*\*

MCZ An2 1w

C -0.310285 0.900337 0.130985  
C -0.802659 2.246445 0.400824  
C -1.218357 -0.264393 0.055016  
C -3.169846 1.931217 0.326147  
C -3.019588 0.957748 -0.881856  
O -4.267827 2.082067 0.868017  
N -2.436244 -0.271209 -0.357149  
N -2.050653 2.614852 0.687125  
C 0.196397 3.289784 0.463634

C 1.533041 3.060086 0.288707  
H 2.257164 3.865406 0.335362  
C 1.982829 1.735195 0.048375  
C 1.062208 0.683985 -0.006220  
H 1.439049 -0.318934 -0.170150  
H -0.174215 4.289768 0.669017  
C -0.700216 -1.587676 0.559468  
C -0.405042 -1.721974 1.926502  
C -0.533577 -2.721799 -0.248164  
C 0.012825 -2.934341 2.472848  
H -0.519331 -0.848563 2.563238  
C -0.106085 -3.943096 0.281041  
C 0.161944 -4.050843 1.645574  
H 0.224427 -3.005548 3.536662  
H 0.018336 -4.795769 -0.379311  
H 0.493170 -5.002113 2.054999  
H -2.325814 1.417404 -1.604564  
Cl -0.813974 -2.648758 -1.986867  
C -4.348842 0.654760 -1.564011  
H -4.197221 -0.065682 -2.376999  
H -5.055400 0.234869 -0.842872  
H -4.786515 1.571323 -1.976773  
N 3.368102 1.477399 -0.124633  
O 4.177284 2.422526 -0.052974  
O 3.745804 0.297813 -0.344706  
O 6.421622 -0.659054 -0.861334  
H 6.029305 -1.513133 -1.094778  
H 5.642624 -0.106855 -0.639754

\*\*\*\*

MCZ An2 2w

C 0.204620 -0.681107 -0.097133  
C 1.055288 -1.856907 -0.006894  
C 0.766088 0.686656 -0.146007  
C 3.224086 -0.925373 -0.322592  
C 2.673126 0.049324 -1.398473  
O 4.403052 -0.815882 0.056456  
N 1.877384 1.043369 -0.685375  
N 2.386801 -1.885552 0.119021  
C 0.384610 -3.131806 0.058747  
C -0.978078 -3.261003 0.032220  
H -1.455290 -4.233324 0.073400  
C -1.781232 -2.095083 -0.041410  
C -1.184266 -0.832958 -0.083205  
H -1.825868 0.039947 -0.116291  
H 1.025352 -4.004941 0.137530  
C -0.000758 1.780154 0.551939  
C -0.162000 1.707684 1.945933  
C -0.533305 2.901975 -0.099952  
C -0.800570 2.716494 2.665113  
H 0.236458 0.839375 2.464240  
C -1.184940 3.918193 0.604863  
C -1.313330 3.827911 1.990787  
H -0.899572 2.633305 3.744285  
H -1.590764 4.766686 0.062826  
H -1.819492 4.620463 2.536494  
H 2.023597 -0.529059 -2.075476  
Cl -0.448125 3.062307 -1.852945  
C 3.770382 0.738215 -2.201909

H 3.323352 1.437963 -2.918174  
H 4.437738 1.291062 -1.535306  
H 4.367588 0.000313 -2.750040  
N -3.200907 -2.211627 -0.061846  
O -3.717452 -3.341812 -0.003270  
O -3.893869 -1.167194 -0.137117  
O -6.780375 -0.945087 -0.307038  
H -6.662210 -0.001278 -0.489055  
H -5.862679 -1.274583 -0.213782  
O 6.001895 -2.036499 2.008161  
H 5.302863 -1.769942 1.364553  
H 6.629760 -1.300956 1.962556

\*\*\*\*

MCZ TS2 0w

C 0.379659 0.566078 -0.048247  
C 1.299565 1.488475 0.497074  
C 0.642200 -0.897373 -0.269168  
C 3.357778 0.193058 0.313819  
C 3.009377 -0.817484 -0.672542  
O 4.578152 0.001819 0.714487  
N 1.752873 -1.434066 -0.642518  
N 2.574467 1.068709 0.956343  
C 0.970347 2.839219 0.662150  
C -0.273972 3.322640 0.275107  
H -0.543719 4.364311 0.398074  
C -1.171287 2.423050 -0.295696  
C -0.863771 1.075700 -0.454670  
H -1.608235 0.416902 -0.884060  
H 1.703162 3.515402 1.094380  
C -0.542146 -1.819271 -0.233328  
C -0.826733 -2.611050 -1.359620  
C -1.372142 -1.974890 0.888506  
C -1.902229 -3.496492 -1.376985  
H -0.177566 -2.517028 -2.224899  
C -2.452341 -2.859343 0.888759  
C -2.721374 -3.617418 -0.250882  
H -2.101311 -4.088549 -2.265954  
H -3.065401 -2.954976 1.779182  
H -3.564618 -4.302661 -0.252432  
H 2.958899 1.512528 1.785304  
H 4.345227 -1.068199 0.101418  
C 3.632150 -0.748750 -2.067751  
H 4.646247 -0.337723 -2.041758  
H 3.678897 -1.757538 -2.491225  
H 3.029103 -0.129419 -2.749331  
Cl -1.043385 -1.089223 2.380047  
N -2.490349 2.910415 -0.733912  
O -3.255374 2.104161 -1.263599  
O -2.749347 4.100452 -0.544392

\*\*\*\*

MCZ TS2 1w

C 0.098535 -0.662943 -0.104558  
C -0.581697 -1.769104 0.447980  
C -0.531714 0.686326 -0.287967  
C -2.953120 -1.153286 0.089344  
C -2.843406 0.045508 -0.686842

O -4.114117 -1.685014 0.319600  
N -1.750348 0.941145 -0.589080  
N -1.929822 -1.685334 0.841265  
C 0.089551 -2.982264 0.664112  
C 1.422370 -3.137671 0.303373  
H 1.946302 -4.072356 0.462824  
C 2.074504 -2.059915 -0.291651  
C 1.433547 -0.837614 -0.484810  
H 1.992823 -0.015429 -0.913892  
H -0.447358 -3.815317 1.110444  
C 0.381695 1.879821 -0.233827  
C 0.470771 2.720716 -1.355619  
C 1.133674 2.229910 0.898527  
C 1.292820 3.846177 -1.359746  
H -0.123873 2.471784 -2.229557  
C 1.957435 3.356924 0.912572  
C 2.041867 4.162649 -0.223213  
H 1.348863 4.472705 -2.245585  
H 2.516839 3.599173 1.810466  
H 2.687527 5.036551 -0.213478  
H -2.258888 -2.414862 1.466434  
H -4.045380 0.599143 0.053580  
O -5.123993 0.462229 0.532726  
H -4.886575 -0.706924 0.424616  
H -5.787492 0.756921 -0.112121  
N 3.474190 -2.207483 -0.705056  
O 4.029109 -3.285228 -0.475119  
O 4.016302 -1.249096 -1.259602  
Cl 1.019845 1.280439 2.379991  
C -3.524807 0.114431 -2.056105  
H -3.835730 1.141524 -2.281539  
H -2.833741 -0.198093 -2.851010  
H -4.399378 -0.541702 -2.101183

\*\*\*\*

MCZ TS2 2w

C 0.115736 0.504976 0.146067  
C -0.810770 1.240344 0.917026  
C 0.006256 -0.971880 -0.024108  
C -2.823185 -0.227210 0.907367  
C -2.412261 -1.202840 -0.043347  
O -4.038401 -0.025467 1.249947  
N -1.081085 -1.648211 -0.130986  
N -1.901993 0.623927 1.550643  
C -0.629132 2.622992 1.104923  
C 0.434745 3.294810 0.518788  
H 0.578852 4.358987 0.661776  
C 1.317968 2.569109 -0.280983  
C 1.171542 1.194858 -0.459277  
H 1.900972 0.660989 -1.056272  
H -1.336697 3.173155 1.720611  
C 1.275481 -1.749519 -0.219528  
C 2.334871 -1.766956 0.702933  
C 1.418993 -2.537177 -1.375355  
C 3.492454 -2.515417 0.480211  
C 2.568904 -3.286667 -1.614945  
C 3.612785 -3.271436 -0.685943  
H 4.283775 -2.507983 1.222930  
H 2.651050 -3.878244 -2.522740

H 4.516404 -3.849321 -0.860150  
H -2.415720 1.248503 2.165126  
H -2.883715 -0.310001 -1.369377  
O -3.481928 0.205214 -2.124392  
H -4.966118 0.118753 0.175911  
O -5.470758 0.324147 -0.749422  
H -4.560738 0.309456 -1.536000  
H -3.547996 -0.374589 -2.902909  
H -5.873828 1.205906 -0.685104  
N 2.430461 3.261983 -0.932420  
O 2.558717 4.472008 -0.720377  
O 3.177640 2.602497 -1.659874  
Cl 2.218475 -0.885545 2.226086  
H 0.598169 -2.549655 -2.086172  
C -3.387293 -2.365863 -0.268829  
H -3.352449 -3.072300 0.571783  
H -4.426015 -2.044938 -0.381768  
H -3.096422 -2.918279 -1.168821

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