

## Supplementary Information

# Crystal Phase Transition of Urea: What Governs the Reaction Kinetics in Molecular Crystal Phase Transition

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#### 1. Other crystal structures for urea

In Fig. S1, we show further 8 urea crystal structures, including phase **IV** and **III** mentioned in the manuscript (Crystal **A** to **C** are shown in Fig. 2) and crystal **D**, **E**, **F**, **G**, **H** and **J** that are within 1 kcal/mol per molecule from the GM (calculated by DFT). The properties of Crystal **D**, **E**, **F**, **G**, **H** and **J** are summarized in Table S1.

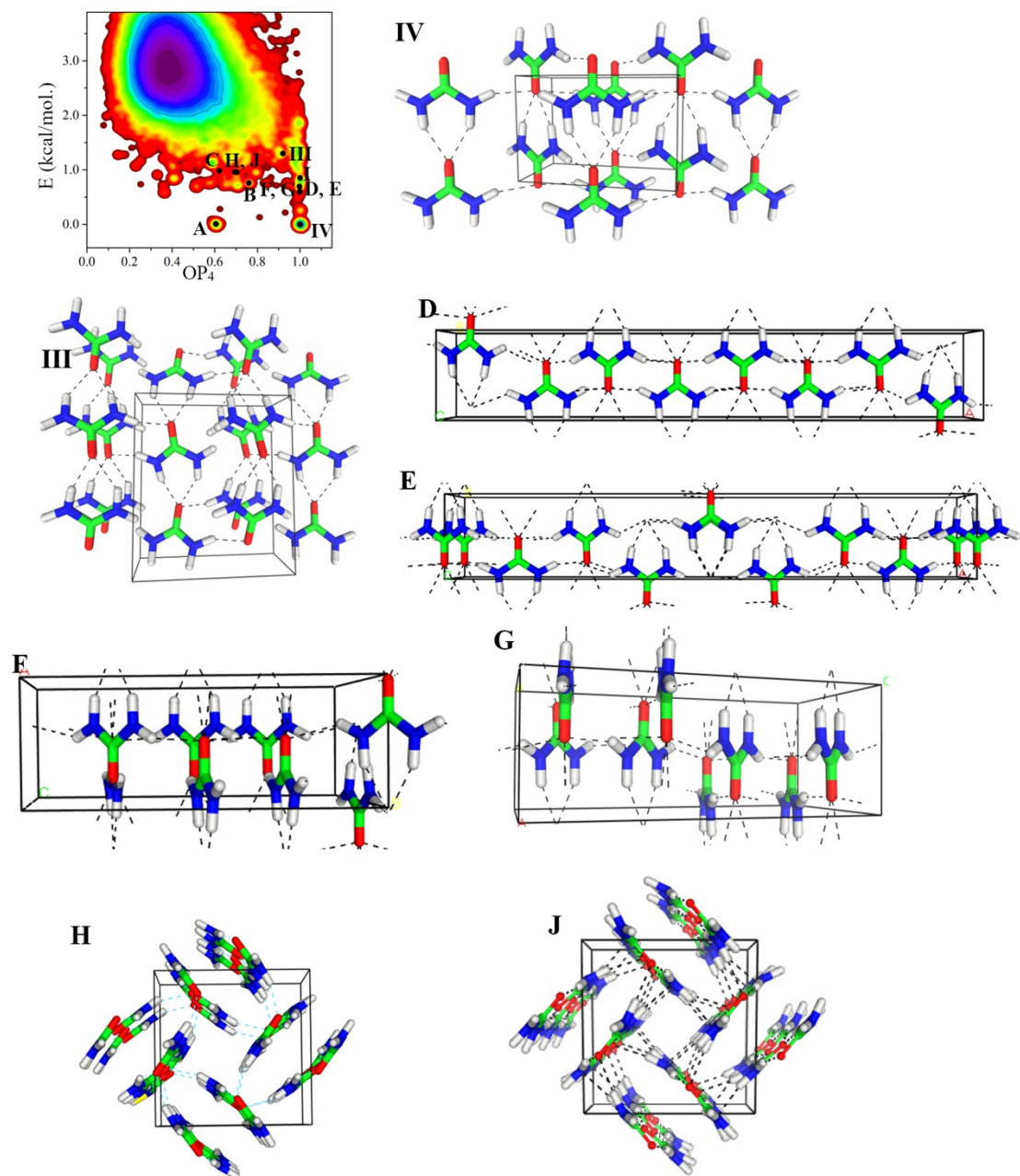
**Table S1:** Six metastable crystal structures of urea<sup>§</sup>.

Phase	S.G.	Vol.	N <sub>H-bond</sub> *	E
<b>D</b>	P2	77.3	4 (I+II)	0.80
<b>E</b>	P2 <sub>1</sub>	77.3	4 (I+II)	0.81
<b>F</b>	P2	78.4	4 (I+II)	0.64
<b>G</b>	P2/c	77.0	4 (I+II)	0.75
<b>H</b>	P <sup>4</sup> <sub>21</sub> c	77.4	2 (III)	0.79
<b>J</b>	P2 <sub>1</sub> /c	77.3	2 (III)	0.65

<sup>§</sup>Listed data includes the symmetry group (S.G.), the volume (Å<sup>3</sup>/mole.), the average number of H<sub>bond</sub> per molecule (N<sub>H-bond</sub>) and the relative energy (E) with reference to the GM (phase **III**). All

energies are in the unit of kcal/mol per molecule.

\*Roman number in parenthesis describes the  $H_{\text{bond}}$  network pattern in Fig. 1 of the manuscript.



**Figure S1:** Crystal structures of low energy urea crystals. The 12 crystals are labelled in the upper left global PES.

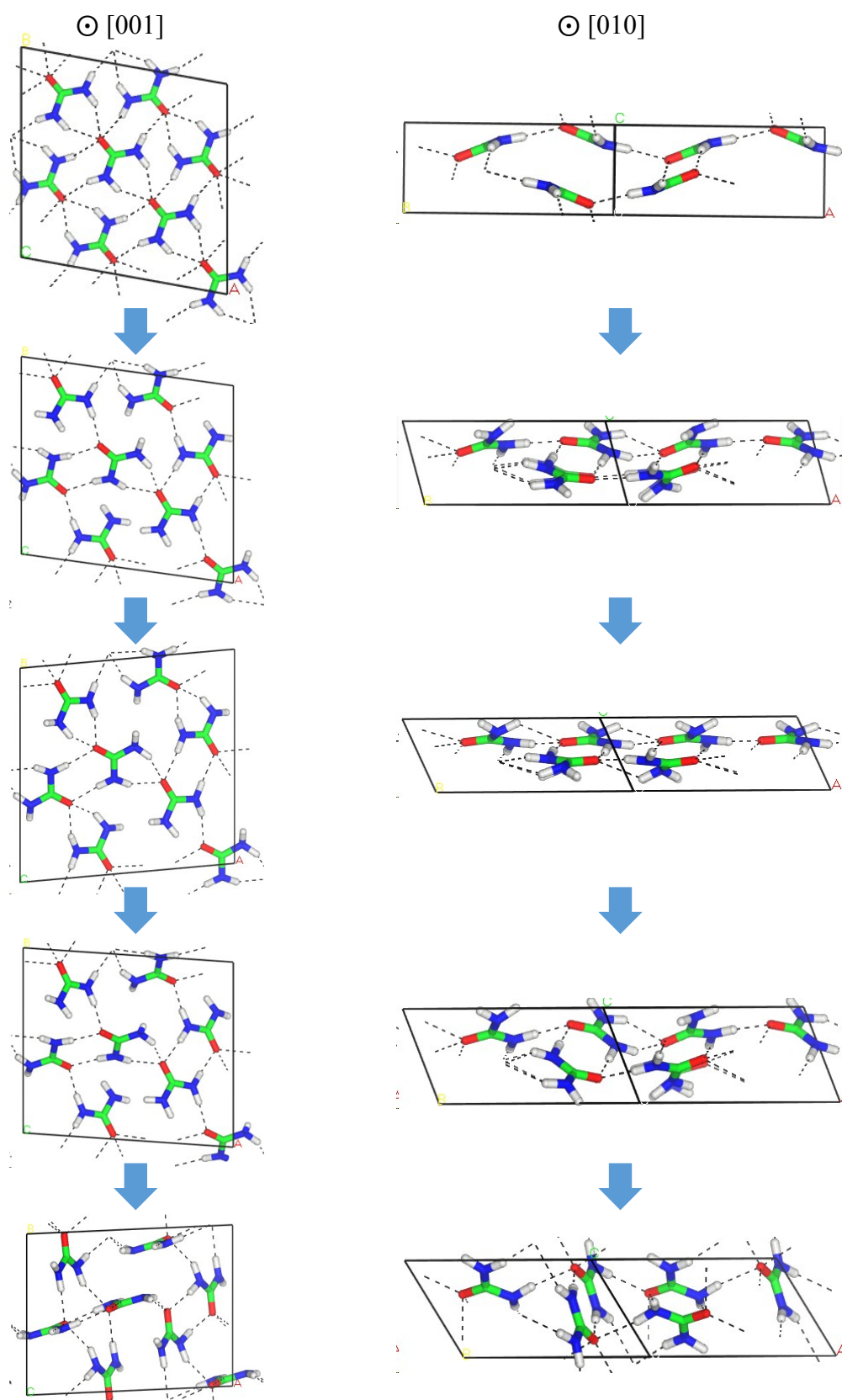
## 2. Barriers to transform to crystal A that calculated using Amber force field.

**Table S2:** Barriers to transform to crystal A that calculated using Amber force field.

Phase	$E_a$
<b>IV</b>	---
<b>A</b>	0.30
<b>B</b>	2.24
<b>I</b>	0.14
<b>C</b>	0.39
<b>III</b>	0.01

## 3. Pathway for the transformation from crystal C to B

Crystal **C** has a different hydrogen network (only Type-III) from the other low energy crystal structures (generally containing Type-I network), and thus has been found to have a high barrier to transit to other low energy crystals (see Fig. 3). In Figure S2, we show the reaction snapshots in the lowest energy pathway from crystal **C** to **B**. We noticed that a large atomic movement are required in the reaction, where 50%  $H_{\text{bond}}$  in Crystal **C** breaks at the TS (Fig. S2). The barrier of the transformation is 2.24 kcal/mol per molecule (Fig. 3).



**Figure S2:** Reaction snapshots from Crystal B to C in the lowest energy pathway. Two view angles, [001] and [010] with reference to crystal D lattice, are shown.

#### 4. PES of 16 urea molecules per unit cell.

We have also done a SSW search based on urea crystals with 16 molecules per unit cell.  $10^5$  minima are visited in total in 10 parallel runs. The main features of the PES obtained from 8-molecule crystals are reserved in in this figure, including the solid-liquid boundary at 1.5 kcal/mol and many solid phases along the  $OP_4=1.0$  region. Due to system scale, less crystal phases are observed within  $10^5$  steps, making this figure sparse compare to Fig. 2bin the manuscript.

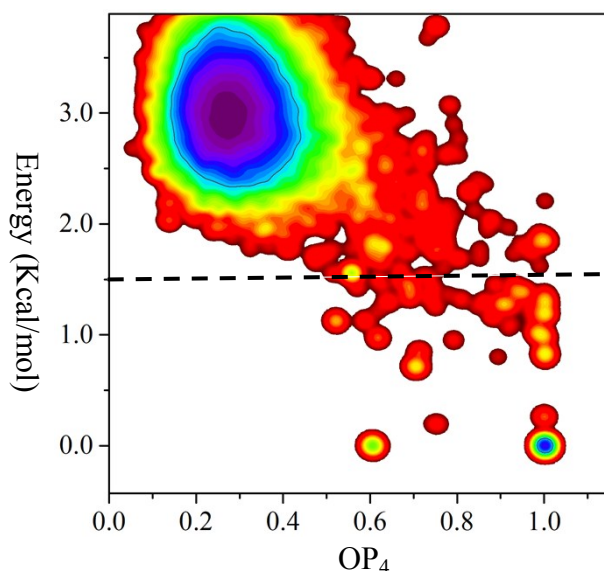


Figure S3. The PES of urea crystals with 16 molecules per unit cell.

#### 5. Structure information for urea crystal structures in .arc format.

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N 0.877320571 1.514632314 3.335923128 CORE 3 N N 0.0000 3
N 5.398924280 1.513983264 1.833901360 CORE 4 N N 0.0000 4
H 2.326188014 2.289807148 0.823111131 CORE 5 H H 0.0000 5
H 3.949319904 2.298042690 4.347296936 CORE 6 H H 0.0000 6
H 0.811088936 2.518955456 3.406962640 CORE 7 H H 0.0000 7
H 5.464465829 2.518133989 1.761712185 CORE 8 H H 0.0000 8
H 1.621537531 3.786169667 1.356988383 CORE 9 H H 0.0000 9
H 4.655883778 3.794329031 3.815155401 CORE 10 H H 0.0000 10
H 1.517491545 1.022787272 3.940902550 CORE 11 H H 0.0000 11
H 4.759116196 1.021614115 1.228862984 CORE 12 H H 0.0000 12
C 3.138595456 4.000847550 0.000365937 CORE 13 C C 0.0000 13
C 0.000204322 0.806998001 2.584938991 CORE 14 C C 0.0000 14
O 3.139361727 0.464444847 0.000433953 CORE 15 O O 0.0000 15
O 0.000962475 4.343406607 2.585061151 CORE 16 O O 0.0000 16
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end
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N    1.246800720  3.073282107  3.151213391 CORE  2 N N  0.0000  2
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C    8.659265405  5.768304876  0.804688976 CORE 28 C C  0.0000 28
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O    4.062517328  1.922699944  2.432320186 CORE 31 O O  0.0000 31
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H    0.911222134  3.586994182  1.886214207 CORE  4 H H  0.0000  4
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C    4.124101662  3.515866413  1.985735691 CORE  8 C C  0.0000  8
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Crystal D  
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H	1.422554696	1.439454234	8.207551868	CORE	24	H	H	0.0000	24
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H	0.637877507	0.066428705	2.305186376	CORE	24	H	H	0.0000	24
H	3.443745872	3.097865163	0.863537530	CORE	25	H	H	0.0000	25
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O	0.978535961	5.268426508	3.896843496	CORE	30	O	O	0.0000	30
O	-0.550417664	1.742962765	0.335325045	CORE	31	O	O	0.0000	31
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Crystal F  
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N	0.869222272	5.359453386	1.229063295	CORE	7	N	N	0.0000	7
N	3.598564643	3.150190661	3.204370111	CORE	8	N	N	0.0000	8
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H	4.162518555	0.864990183	2.381566513	CORE	10	H	H	0.0000	10
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H	4.771945143	5.120877058	1.568132258	CORE	12	H	H	0.0000	12
H	0.021502225	1.469869741	2.397222028	CORE	13	H	H	0.0000	13
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H	3.258446241	4.034384073	3.568716749	CORE	24	H	H	0.0000	24
C	1.739662269	6.189376112	0.617609037	CORE	25	C	C	0.0000	25
C	2.727905306	2.320646001	2.592809981	CORE	26	C	C	0.0000	26
C	7.195466382	1.933943286	3.331613999	CORE	27	C	C	0.0000	27
C	6.207084393	6.576081811	1.357035380	CORE	28	C	C	0.0000	28
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O	1.561799667	2.670186755	2.271134665	CORE	30	O	O	0.0000	30
O	6.029370153	1.584366715	3.653316144	CORE	31	O	O	0.0000	31
O	7.373229491	6.925145379	1.678720495	CORE	32	O	O	0.0000	32

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Crystal G  
!BIOSYM archive 2  
PBC=ON

!DATE

PBC	28.4254	4.7648	4.5683	90.0013	89.9991	89.9167			
N	15.010667679	3.839817386	3.839370669	CORE	1	N	N	0.0000	1
N	13.421708083	0.924668042	1.555214001	CORE	2	N	N	0.0000	2
H	15.101839145	0.071863673	3.714413558	CORE	3	H	H	0.0000	3
H	13.330545829	4.692587068	1.430327462	CORE	4	H	H	0.0000	4
H	14.325954209	3.351967083	3.283685806	CORE	5	H	H	0.0000	5
H	14.106471144	1.412561877	0.999572063	CORE	6	H	H	0.0000	6
C	15.975024073	3.125909274	4.472369876	CORE	7	C	C	0.0000	7
C	12.457374042	1.638513251	2.188232226	CORE	8	C	C	0.0000	8
N	16.948962803	3.836498141	0.527864204	CORE	9	N	N	0.0000	9
N	11.483441194	0.928007354	2.812007891	CORE	10	N	N	0.0000	10
H	16.847073297	0.068800105	0.654894876	CORE	11	H	H	0.0000	11
H	11.585265606	4.695743167	2.939022647	CORE	12	H	H	0.0000	12
H	17.621365153	3.345700747	1.095433125	CORE	13	H	H	0.0000	13
H	10.810986036	1.418825222	3.379625612	CORE	14	H	H	0.0000	14
O	15.968862035	1.862390918	4.478852680	CORE	15	O	O	0.0000	15
O	12.463470468	2.902066243	2.194740206	CORE	16	O	O	0.0000	16
N	22.071959890	3.841415675	3.745610397	CORE	17	N	N	0.0000	17
N	6.360470238	0.923217947	1.461644568	CORE	18	N	N	0.0000	18
H	22.154370635	0.078338338	3.660232157	CORE	19	H	H	0.0000	19
H	6.277977048	4.686334755	1.376136916	CORE	20	H	H	0.0000	20
H	21.322794341	3.372785266	3.259796273	CORE	21	H	H	0.0000	21

H	7.109495295	1.392018458	0.975566369	CORE	22	H	H	0.0000	22
C	22.966032242	3.115870181	4.456047130	CORE	23	C	C	0.0000	23
C	5.466285982	1.648787192	2.171864248	CORE	24	C	C	0.0000	24
N	23.983220069	3.817780982	0.480263155	CORE	25	N	N	0.0000	25
N	4.448807627	0.946978479	2.764045518	CORE	26	N	N	0.0000	26
H	23.848863673	0.042521686	0.648058560	CORE	27	H	H	0.0000	27
H	4.583594371	4.722367071	2.932225560	CORE	28	H	H	0.0000	28
H	24.527039984	3.313693417	1.160400077	CORE	29	H	H	0.0000	29
H	3.905359762	1.451026082	3.444575837	CORE	30	H	H	0.0000	30
O	22.893054038	1.861694553	4.543808034	CORE	31	O	O	0.0000	31
O	5.539258027	2.902966632	2.259737836	CORE	32	O	O	0.0000	32
N	20.424728854	0.913388397	1.531017880	CORE	33	N	N	0.0000	33
N	8.007661386	3.851243491	3.815129950	CORE	34	N	N	0.0000	34
H	20.334155345	4.679100730	1.426092856	CORE	35	H	H	0.0000	35
H	8.098142197	0.085505644	3.710222626	CORE	36	H	H	0.0000	36
H	21.134964300	1.392216693	0.996795128	CORE	37	H	H	0.0000	37
H	7.297365604	3.372440486	3.281001850	CORE	38	H	H	0.0000	38
C	19.479274350	1.631970939	2.182172109	CORE	39	C	C	0.0000	39
C	8.953180649	3.132574930	4.466242409	CORE	40	C	C	0.0000	40
N	18.500872577	0.928320224	2.807711310	CORE	41	N	N	0.0000	41
N	9.931491221	3.836295698	0.523596125	CORE	42	N	N	0.0000	42
H	18.600023515	4.696271259	2.937182478	CORE	43	H	H	0.0000	43
H	9.832319315	0.068420530	0.653009944	CORE	44	H	H	0.0000	44
H	17.838351277	1.422367623	3.384232914	CORE	45	H	H	0.0000	45
H	10.593968472	3.342267518	1.100040871	CORE	46	H	H	0.0000	46
O	19.498273949	2.896589764	2.199200963	CORE	47	O	O	0.0000	47
O	8.934071870	1.868021183	4.483200556	CORE	48	O	O	0.0000	48
N	27.580052308	1.478556110	1.442724951	CORE	49	N	N	0.0000	49
N	0.852323354	3.286258324	3.726682414	CORE	50	N	N	0.0000	50
H	27.489780323	2.480746402	1.364087129	CORE	51	H	H	0.0000	51
H	0.942504621	2.284013986	3.648104463	CORE	52	H	H	0.0000	52
H	28.333422093	1.011177996	0.958815808	CORE	53	H	H	0.0000	53
H	0.098766913	3.753639771	3.243069906	CORE	54	H	H	0.0000	54
C	26.696705125	0.755367293	2.167280286	CORE	55	C	C	0.0000	55
C	1.735534162	4.009422983	4.451358929	CORE	56	C	C	0.0000	56
N	25.685709619	1.458044728	2.769296733	CORE	57	N	N	0.0000	57
N	2.746298109	3.306814151	0.485449566	CORE	58	N	N	0.0000	58
H	25.817023802	2.446657076	2.939684396	CORE	59	H	H	0.0000	59
H	2.615458102	2.318105018	0.655332253	CORE	60	H	H	0.0000	60
H	25.143615573	0.954117942	3.450867898	CORE	61	H	H	0.0000	61
H	3.288828945	3.810639022	1.166673558	CORE	62	H	H	0.0000	62
O	26.777796462	4.265540848	2.258028326	CORE	63	O	O	0.0000	63
O	1.654585246	0.499263495	4.541982920	CORE	64	O	O	0.0000	64

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Crystal H  
!BIOSYM archive 2  
PBC=ON

!DATE

PBC	28.4088	4.7694	4.5636	89.9967	89.9440	89.9978			
N	27.441379548	3.016464418	3.939875650	CORE	1	N	N	0.0000	1
N	0.971640614	3.016061948	0.624245278	CORE	2	N	N	0.0000	2
H	27.539823916	4.013102735	3.811370040	CORE	3	H	H	0.0000	3
H	0.872973039	4.012655348	0.752747918	CORE	4	H	H	0.0000	4
H	26.764073085	2.527167753	3.376864101	CORE	5	H	H	0.0000	5
H	1.648713889	2.526931146	1.187643274	CORE	6	H	H	0.0000	6

C	28.408571449	2.302857263	0.000278986	CORE	7	C	0.0000	7
O	28.408435359	1.039694617	0.000122357	CORE	8	O	0.0000	8
N	6.099410417	3.026057201	3.833563282	CORE	9	N	0.0000	9
N	22.314428720	3.025884620	0.729922771	CORE	10	N	0.0000	10
H	6.185242068	4.027262708	3.740414527	CORE	11	H	0.0000	11
H	22.228539119	4.027089757	0.823351229	CORE	12	H	0.0000	12
H	5.356340966	2.550662059	3.344938453	CORE	13	H	0.0000	13
H	23.057232734	2.550631443	1.218896905	CORE	14	H	0.0000	14
C	7.000451134	2.308493198	4.543601853	CORE	15	C	0.0000	15
C	21.412947778	2.308202776	0.020548184	CORE	16	C	0.0000	16
N	8.006031764	3.017848385	0.571925217	CORE	17	N	0.0000	17
N	20.407041858	3.018221387	3.992793483	CORE	18	N	0.0000	18
H	7.880797566	4.009838169	0.726267820	CORE	19	H	0.0000	19
H	20.532725730	4.010004250	3.837807347	CORE	20	H	0.0000	20
H	8.558420468	2.520565605	1.249739152	CORE	21	H	0.0000	21
H	19.854603629	2.520799092	3.315086971	CORE	22	H	0.0000	22
O	6.931815966	1.052890894	0.067530519	CORE	23	O	0.0000	23
O	21.481465000	1.053192304	4.496738654	CORE	24	O	0.0000	24
N	4.461285927	0.094281971	1.610699446	CORE	25	N	0.0000	25
N	23.951555838	0.094652626	2.952993653	CORE	26	N	0.0000	26
H	4.365808440	3.864135097	1.506771308	CORE	27	H	0.0000	27
H	24.047290036	3.864534090	3.056964583	CORE	28	H	0.0000	28
H	5.169937604	0.574787566	1.076111606	CORE	29	H	0.0000	29
H	23.243075646	0.575449858	3.487623292	CORE	30	H	0.0000	30
C	3.519168456	0.811576215	2.267820908	CORE	31	C	0.0000	31
C	24.894048283	0.811886688	2.296251861	CORE	32	C	0.0000	32
N	2.546886804	0.105531176	2.899857936	CORE	33	N	0.0000	33
N	25.866087201	0.105697089	1.664211098	CORE	34	N	0.0000	34
H	2.642429082	3.877856358	3.027098957	CORE	35	H	0.0000	35
H	25.770973771	3.878055198	1.536925830	CORE	36	H	0.0000	36
H	1.886170630	0.598530633	3.478943647	CORE	37	H	0.0000	37
H	26.527291026	0.598524177	1.085350253	CORE	38	H	0.0000	38
O	3.536105788	2.076295062	2.284571111	CORE	39	O	0.0000	39
O	24.877472395	2.076626152	2.279948219	CORE	40	O	0.0000	40
N	11.641598755	0.726671714	1.582436348	CORE	41	N	0.0000	41
N	16.771833783	0.725955115	2.981605303	CORE	42	N	0.0000	42
H	11.552087912	1.726182211	1.476473800	CORE	43	H	0.0000	43
H	16.861467865	1.725496129	3.087444129	CORE	44	H	0.0000	44
H	12.378136430	0.247150322	1.088335470	CORE	45	H	0.0000	45
H	16.035133290	0.246881939	3.475888784	CORE	46	H	0.0000	46
C	10.726600818	0.011627088	2.278261549	CORE	47	C	0.0000	47
C	17.686836126	0.010687635	2.285997937	CORE	48	C	0.0000	48
N	9.715064538	0.728596394	2.860557849	CORE	49	N	0.0000	49
N	18.698428697	0.727578441	1.703731923	CORE	50	N	0.0000	50
H	9.852210963	1.716956698	3.029279484	CORE	51	H	0.0000	51
H	18.561743705	1.716000793	1.535208405	CORE	52	H	0.0000	52
H	9.144200612	0.233594595	3.524776889	CORE	53	H	0.0000	53
H	19.269598882	0.232298100	1.039962598	CORE	54	H	0.0000	54
O	10.783114290	3.526187121	2.364227915	CORE	55	O	0.0000	55
O	17.630617737	3.525257622	2.200039088	CORE	56	O	0.0000	56
N	13.249857854	2.570318663	3.922735866	CORE	57	N	0.0000	57
N	15.163877291	2.569924218	0.641192038	CORE	58	N	0.0000	58
H	13.344631446	1.571773539	3.810001471	CORE	59	H	0.0000	59
H	15.069094066	1.571401567	0.753917775	CORE	60	H	0.0000	60
H	12.554083592	3.054757765	3.375301355	CORE	61	H	0.0000	61
H	15.859571685	3.054416780	1.188701254	CORE	62	H	0.0000	62
C	14.204651215	3.281084469	0.000221644	CORE	63	C	0.0000	63
O	14.204702085	4.547059598	0.000365339	CORE	64	O	0.0000	64

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Crystal I  
!BIOSYM archive 2  
PBC=ON

!DATE

PBC	4.7743	16.3554	8.1946	78.5497	89.9978	90.0022		
N	3.308612113	14.512658814	5.775963213	CORE	1 N N	0.0000	1	
N	3.309622189	3.471702136	2.257896964	CORE	2 N N	0.0000	2	
H	4.314375709	14.553417456	5.846889282	CORE	3 H H	0.0000	3	
H	4.315351228	3.430706757	2.186423780	CORE	4 H H	0.0000	4	
H	2.816828353	15.302422249	5.394715661	CORE	5 H H	0.0000	5	
H	2.817909632	2.681765396	2.638775082	CORE	6 H H	0.0000	6	
C	2.607582505	13.450230188	6.241422550	CORE	7 C C	0.0000	7	
C	2.608240444	4.533213100	1.790955123	CORE	8 C C	0.0000	8	
N	3.323848129	12.411774453	6.732102350	CORE	9 N N	0.0000	9	
N	3.324084897	5.571472177	1.299209004	CORE	10 N N	0.0000	10	
H	4.327809633	12.380130282	6.632302767	CORE	11 H H	0.0000	11	
H	4.328039973	5.603423002	1.399096117	CORE	12 H H	0.0000	12	
H	2.837056538	11.589510015	7.055136961	CORE	13 H H	0.0000	13	
H	2.836943493	6.393286213	0.975508758	CORE	14 H H	0.0000	14	
O	1.341748226	13.435073177	6.226136331	CORE	15 O O	0.0000	15	
O	1.342381257	4.547714876	1.805717286	CORE	16 O O	0.0000	16	
N	2.191308590	2.671925466	7.541965015	CORE	17 N N	0.0000	17	
N	2.190080855	15.311994826	0.491498869	CORE	18 N N	0.0000	18	
H	1.185994004	2.712663735	7.621291432	CORE	19 H H	0.0000	19	
H	1.184788855	15.271567636	0.411641303	CORE	20 H H	0.0000	20	
H	2.683740454	3.474084897	7.189673388	CORE	21 H H	0.0000	21	
H	2.682241695	14.509424473	0.843244418	CORE	22 H H	0.0000	22	
C	2.900231560	0.000715112	0.000851861	CORE	23 C C	0.0000	23	
O	4.165219800	0.000593445	0.000896271	CORE	24 O O	0.0000	24	
N	0.308080499	12.961734722	3.340673430	CORE	25 N N	0.0000	25	
N	0.309660433	5.024582729	4.691412914	CORE	26 N N	0.0000	26	
H	4.081677292	13.087047655	3.307252377	CORE	27 H H	0.0000	27	
H	4.083293219	4.898565700	4.725047389	CORE	28 H H	0.0000	28	
H	0.798750486	13.144397861	4.202745343	CORE	29 H H	0.0000	29	
H	0.800398132	4.841284016	3.829539577	CORE	30 H H	0.0000	30	
C	1.013502486	12.697684495	2.215603057	CORE	31 C C	0.0000	31	
C	1.015105987	5.286641265	5.817004450	CORE	32 C C	0.0000	32	
N	0.295887104	12.538384173	1.070197357	CORE	33 N N	0.0000	33	
N	0.297352055	5.445129540	6.962305205	CORE	34 N N	0.0000	34	
H	4.071574066	12.393975594	1.121679493	CORE	35 H H	0.0000	35	
H	4.073034163	5.589673287	6.911080388	CORE	36 H H	0.0000	36	
H	0.778869143	12.199374295	0.252139215	CORE	37 H H	0.0000	37	
H	0.780851191	5.782679605	7.780608587	CORE	38 H H	0.0000	38	
O	2.275247407	12.625676056	2.221921548	CORE	39 O O	0.0000	39	
O	2.276887292	5.358339090	5.811288189	CORE	40 O O	0.0000	40	
N	0.425206707	0.687966555	2.868163357	CORE	41 N N	0.0000	41	
N	0.424613935	17.297357059	5.164309767	CORE	42 N N	0.0000	42	
H	1.419654496	16.875984440	2.920265475	CORE	43 H H	0.0000	43	
H	1.420451300	1.108586677	5.112838991	CORE	44 H H	0.0000	44	
H	4.713913507	16.763616601	2.028910246	CORE	45 H H	0.0000	45	
H	4.714270534	1.220483884	6.003757139	CORE	46 H H	0.0000	46	
C	4.480410838	0.814576875	4.016342762	CORE	47 C C	0.0000	47	
O	3.219459717	0.814361569	4.016526205	CORE	48 O O	0.0000	48	
N	3.308035564	7.938005999	4.487343420	CORE	49 N N	0.0000	49	

N	3.307495506	10.046760978	3.545235850	CORE	50	N	N	0.0000	50
H	4.310119701	7.895957387	4.374591305	CORE	51	H	H	0.0000	51
H	4.309549854	10.089124818	3.657801883	CORE	52	H	H	0.0000	52
H	2.817233729	7.117079826	4.809217244	CORE	53	H	H	0.0000	53
H	2.816180872	10.867397991	3.223367616	CORE	54	H	H	0.0000	54
C	2.599934437	8.992276238	4.016404272	CORE	55	C	C	0.0000	55
O	1.332970086	8.992243346	4.016633639	CORE	56	O	O	0.0000	56
N	0.313224778	9.465843111	6.928179666	CORE	57	N	N	0.0000	57
N	0.313218999	8.518338054	1.104325547	CORE	58	N	N	0.0000	58
H	4.081543238	9.391933276	6.950580119	CORE	59	H	H	0.0000	59
H	4.081557924	8.592467932	1.082172644	CORE	60	H	H	0.0000	60
H	0.803527341	9.234853531	6.078090646	CORE	61	H	H	0.0000	61
H	0.803625905	8.748471418	1.954572832	CORE	62	H	H	0.0000	62
C	1.019243173	8.178461742	0.000449288	CORE	63	C	C	0.0000	63
O	2.286629907	8.178000037	0.000461301	CORE	64	O	O	0.0000	64

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Crystal J  
!BIOSYM archive 2  
PBC=ON

!DATE

PBC	4.7937	8.3427	15.4375	94.3284	89.9995	89.9953			
N	0.087868326	5.263162534	13.532399760	CORE	1	N	N	0.0000	1
N	0.088321444	5.503068734	9.556606768	CORE	2	N	N	0.0000	2
N	4.710520696	1.914174938	1.859810523	CORE	3	N	N	0.0000	3
N	4.710069461	1.674151687	5.835806968	CORE	4	N	N	0.0000	4
H	1.082339913	5.235965829	13.354744291	CORE	5	H	H	0.0000	5
H	1.082809454	5.530775404	9.734485676	CORE	6	H	H	0.0000	6
H	3.716090937	1.941343113	2.037597962	CORE	7	H	H	0.0000	7
H	3.715597173	1.646441527	5.657869366	CORE	8	H	H	0.0000	8
H	4.405536510	6.136785686	13.366737224	CORE	9	H	H	0.0000	9
H	4.405455598	4.629702438	9.722538360	CORE	10	H	H	0.0000	10
H	0.392980758	1.040483945	2.025426593	CORE	11	H	H	0.0000	11
H	0.392970246	2.547541968	5.669799513	CORE	12	H	H	0.0000	12
C	4.154754129	4.112722137	13.448766132	CORE	13	C	C	0.0000	13
C	4.155370769	6.653565634	9.639975404	CORE	14	C	C	0.0000	14
C	0.643646306	3.064506526	1.943500856	CORE	15	C	C	0.0000	15
C	0.643055299	0.523753047	5.752267672	CORE	16	C	C	0.0000	16
N	0.066262067	2.954964355	13.465600991	CORE	17	N	N	0.0000	17
N	0.066301718	-0.531461378	9.623155567	CORE	18	N	N	0.0000	18
N	4.732335614	4.222285073	1.926701063	CORE	19	N	N	0.0000	19
N	4.732280997	7.708726465	5.769177781	CORE	20	N	N	0.0000	20
H	1.060101431	2.957280622	13.639382477	CORE	21	H	H	0.0000	21
H	1.060048623	-0.533413641	9.449253742	CORE	22	H	H	0.0000	22
H	3.738422979	4.219972862	1.753018843	CORE	23	H	H	0.0000	23
H	3.738477855	7.710631291	5.943055502	CORE	24	H	H	0.0000	24
H	4.367592947	2.076384151	13.502206000	CORE	25	H	H	0.0000	25
H	4.368145678	0.347414645	9.586576238	CORE	26	H	H	0.0000	26
H	0.430924308	5.100947576	1.890216835	CORE	27	H	H	0.0000	27
H	0.430394087	6.829845700	5.805455998	CORE	28	H	H	0.0000	28
O	2.895507991	4.124763271	13.373013049	CORE	29	O	O	0.0000	29
O	2.896153800	6.641795557	9.716139001	CORE	30	O	O	0.0000	30
O	1.902979962	3.052362938	2.019240837	CORE	31	O	O	0.0000	31
O	1.902310390	0.535610202	5.675924505	CORE	32	O	O	0.0000	32
N	1.958612789	1.983615398	8.592855718	CORE	33	N	N	0.0000	33
N	1.958083300	0.440079322	14.495530768	CORE	34	N	N	0.0000	34

N	2.840141412	5.193981330	6.799117324	CORE	35	N	N	0.0000	35
N	2.840693243	6.737120240	0.896547681	CORE	36	N	N	0.0000	36
H	0.962432759	2.129780720	8.520186122	CORE	37	H	H	0.0000	37
H	0.961754515	0.294207537	14.567925581	CORE	38	H	H	0.0000	38
H	3.836263298	5.047765762	6.871983727	CORE	39	H	H	0.0000	39
H	3.836987613	6.882823862	0.824053950	CORE	40	H	H	0.0000	40
H	2.463970486	1.737600106	7.759550814	CORE	41	H	H	0.0000	41
H	2.463236275	0.686154206	15.328953037	CORE	42	H	H	0.0000	42
H	2.334625876	5.439889133	7.632312406	CORE	43	H	H	0.0000	43
H	2.335397434	6.490953808	0.063295086	CORE	44	H	H	0.0000	44
C	2.656961612	2.474433934	9.651966638	CORE	45	C	C	0.0000	45
C	2.656589288	-0.050794274	13.436608293	CORE	46	C	C	0.0000	46
C	2.141776479	4.702765210	5.740072067	CORE	47	C	C	0.0000	47
C	2.142198272	7.228013089	1.955644811	CORE	48	C	C	0.0000	48
N	1.930436102	2.939003917	10.695607179	CORE	49	N	N	0.0000	49
N	1.930200900	-0.515568319	12.392955486	CORE	50	N	N	0.0000	50
N	2.868474259	4.238248070	4.696469530	CORE	51	N	N	0.0000	51
N	2.868762404	7.692466769	2.999321645	CORE	52	N	N	0.0000	52
H	0.931901049	2.794562611	10.731808015	CORE	53	H	H	0.0000	53
H	0.931747193	-0.370844885	12.356447095	CORE	54	H	H	0.0000	54
H	3.866986034	4.382725615	4.660311963	CORE	55	H	H	0.0000	55
H	3.867201905	7.547861687	3.035725776	CORE	56	H	H	0.0000	56
H	2.405847498	3.234519627	11.536059940	CORE	57	H	H	0.0000	57
H	2.405656829	-0.811052837	11.552601705	CORE	58	H	H	0.0000	58
H	2.393166707	3.942631585	3.856061576	CORE	59	H	H	0.0000	59
H	2.393380260	7.988115685	3.839634832	CORE	60	H	H	0.0000	60
O	3.920363918	2.486012939	9.658441359	CORE	61	O	O	0.0000	61
O	3.920072548	-0.062859550	13.430117239	CORE	62	O	O	0.0000	62
O	0.878413301	4.691017820	5.733631343	CORE	63	O	O	0.0000	63
O	0.878754952	7.240143560	1.962187490	CORE	64	O	O	0.0000	64

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Crystal K

!BIOSYM archive 2

PBC=ON

!DATE

PBC	9.0923	9.0923	7.4917	89.9994	90.0007	89.9992			
N	0.084866699	2.275732812	0.306480390	CORE	1	N	N	0.0000	1
N	9.006534853	6.813583166	0.306587258	CORE	2	N	N	0.0000	2
N	2.276593426	9.005589299	7.189761309	CORE	3	N	N	0.0000	3
N	6.814590633	0.083951952	7.189739108	CORE	4	N	N	0.0000	4
N	4.460350559	6.821781612	3.443879635	CORE	5	N	N	0.0000	5
N	4.631068576	2.267610279	3.443882977	CORE	6	N	N	0.0000	6
N	2.268445513	4.459343270	4.052481507	CORE	7	N	N	0.0000	7
N	6.822923326	4.630102195	4.052304719	CORE	8	N	N	0.0000	8
H	0.896760910	1.681062695	0.273759859	CORE	9	H	H	0.0000	9
H	8.194651834	7.408262669	0.273909615	CORE	10	H	H	0.0000	10
H	1.682107264	8.193503933	7.222300525	CORE	11	H	H	0.0000	11
H	7.409129603	0.896005102	7.222267433	CORE	12	H	H	0.0000	12
H	3.648274092	6.227300306	3.476466993	CORE	13	H	H	0.0000	13
H	5.443103360	2.862126294	3.476413363	CORE	14	H	H	0.0000	14
H	2.863104370	3.647426681	4.019763601	CORE	15	H	H	0.0000	15
H	6.228280053	5.441996515	4.019587459	CORE	16	H	H	0.0000	16
H	8.837485519	2.684475620	6.931507228	CORE	17	H	H	0.0000	17
H	0.253759167	6.405039650	6.931593132	CORE	18	H	H	0.0000	18
H	2.685329297	0.252571676	0.564791695	CORE	19	H	H	0.0000	19

H	6.406090357	8.836780728	0.564758242	CORE	20	H	H	0.0000	20
H	4.799743883	7.230540286	4.310552609	CORE	21	H	H	0.0000	21
H	4.291630872	1.858918418	4.310601716	CORE	22	H	H	0.0000	22
H	1.859865271	4.798935748	3.185770992	CORE	23	H	H	0.0000	23
H	7.231571907	4.290459415	3.185653541	CORE	24	H	H	0.0000	24
C	8.627891056	2.651925191	1.489455585	CORE	25	C	C	0.0000	25
C	0.463493826	6.437397523	1.489566465	CORE	26	C	C	0.0000	26
C	2.652950000	0.462551189	6.006816443	CORE	27	C	C	0.0000	27
C	6.438324469	8.626884485	6.006824821	CORE	28	C	C	0.0000	28
C	5.009722156	7.198192871	2.260980540	CORE	29	C	C	0.0000	29
C	4.081745615	1.891190479	2.260987325	CORE	30	C	C	0.0000	30
C	1.892218497	5.008651045	5.235441842	CORE	31	C	C	0.0000	31
C	7.199065669	4.080772919	5.235258844	CORE	32	C	C	0.0000	32
N	0.091563308	2.139692245	2.616780260	CORE	33	N	N	0.0000	33
N	8.999851067	6.949739881	2.616911603	CORE	34	N	N	0.0000	34
N	2.140941077	8.998956701	4.879377642	CORE	35	N	N	0.0000	35
N	6.950477345	0.090404035	4.879381196	CORE	36	N	N	0.0000	36
N	4.453815418	6.685985640	1.133584112	CORE	37	N	N	0.0000	37
N	4.637590158	2.403419549	1.133523974	CORE	38	N	N	0.0000	38
N	2.404491928	4.452670533	6.362795929	CORE	39	N	N	0.0000	39
N	6.686722991	4.636785443	6.362575983	CORE	40	N	N	0.0000	40
H	1.016879726	1.735160802	2.581956480	CORE	41	H	H	0.0000	41
H	8.074508933	7.354179732	2.582111793	CORE	42	H	H	0.0000	42
H	1.736281163	8.073675753	4.914142966	CORE	43	H	H	0.0000	43
H	7.355000792	1.015757796	4.914086689	CORE	44	H	H	0.0000	44
H	3.528534844	6.281345317	1.168268896	CORE	45	H	H	0.0000	45
H	5.562915950	2.807893831	1.168219190	CORE	46	H	H	0.0000	46
H	2.808999911	3.527350009	6.327991271	CORE	47	H	H	0.0000	47
H	6.282314399	5.562138551	6.327834139	CORE	48	H	H	0.0000	48
H	8.851681786	2.483419891	3.510304993	CORE	49	H	H	0.0000	49
H	0.239626303	6.605907606	3.510443889	CORE	50	H	H	0.0000	50
H	2.484592565	0.238860675	3.985848688	CORE	51	H	H	0.0000	51
H	6.606779886	8.850515620	3.985884645	CORE	52	H	H	0.0000	52
H	4.786083292	7.029696999	0.240089070	CORE	53	H	H	0.0000	53
H	4.305425423	2.059535403	0.240044599	CORE	54	H	H	0.0000	54
H	2.060705586	4.784798168	7.256325345	CORE	55	H	H	0.0000	55
H	7.030465942	4.304658841	7.256107906	CORE	56	H	H	0.0000	56
O	7.606721924	3.400038866	1.523591425	CORE	57	O	O	0.0000	57
O	1.484639025	5.689233654	1.523713114	CORE	58	O	O	0.0000	58
O	3.401104762	1.483569056	5.972798299	CORE	59	O	O	0.0000	59
O	5.690186985	7.605874408	5.972852297	CORE	60	O	O	0.0000	60
O	6.030801536	7.946297324	2.226987580	CORE	61	O	O	0.0000	61
O	3.060670837	1.142994523	2.227000617	CORE	62	O	O	0.0000	62
O	1.144120108	6.029802369	5.269576910	CORE	63	O	O	0.0000	63
O	7.947145995	3.059569165	5.269392302	CORE	64	O	O	0.0000	64

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Crystal L  
!BIOSYM archive 2  
PBC=ON

!DATE

PBC	7.4754	9.2068	9.1338	90.0000	79.5716	90.0000		
N	6.326955995	9.131267030	2.312599551	CORE	1	N	N	0.0000 1
N	1.975716007	4.528029529	2.179012251	CORE	2	N	N	0.0000 2
N	2.802300340	0.074654377	6.670454249	CORE	3	N	N	0.0000 3
N	7.153526874	4.678002932	6.804011432	CORE	4	N	N	0.0000 4

H	6.294973130	8.333293458	2.928148130	CORE	5	H	H	0.0000	5
H	2.007660042	3.730024639	1.563509882	CORE	6	H	H	0.0000	6
H	2.834293827	0.872597851	6.054883629	CORE	7	H	H	0.0000	7
H	7.121578327	5.476003497	7.419604679	CORE	8	H	H	0.0000	8
H	5.457508200	0.245481257	1.896326939	CORE	9	H	H	0.0000	9
H	2.845089133	4.849001365	2.595343018	CORE	10	H	H	0.0000	10
H	3.671732541	8.960461017	7.086784212	CORE	11	H	H	0.0000	11
H	6.284133262	4.357042344	6.387762259	CORE	12	H	H	0.0000	12
C	7.512023905	0.450067926	1.898781298	CORE	13	C	C	0.0000	13
C	0.790581264	5.053530049	2.592974011	CORE	14	C	C	0.0000	14
C	1.617196903	8.755902456	7.084315512	CORE	15	C	C	0.0000	15
C	8.338619926	4.152500674	6.390198931	CORE	16	C	C	0.0000	16
N	1.163977299	9.081408958	2.386783013	CORE	17	N	N	0.0000	17
N	7.138622458	4.478078376	2.104949184	CORE	18	N	N	0.0000	18
N	7.965271670	0.124501388	6.596223528	CORE	19	N	N	0.0000	19
N	1.990607576	4.727916337	6.878084917	CORE	20	N	N	0.0000	20
H	1.121423762	8.143312907	2.758474369	CORE	21	H	H	0.0000	21
H	7.181223960	3.539997546	1.733191732	CORE	22	H	H	0.0000	22
H	8.007796516	1.062587874	6.224530023	CORE	23	H	H	0.0000	23
H	1.947992965	5.666020585	7.249896146	CORE	24	H	H	0.0000	24
H	2.052367398	0.199910303	2.020534207	CORE	25	H	H	0.0000	25
H	6.250252641	4.803370902	2.471142301	CORE	26	H	H	0.0000	26
H	7.076865625	9.005997701	6.962492999	CORE	27	H	H	0.0000	27
H	2.878964225	4.402634374	6.511938718	CORE	28	H	H	0.0000	28
O	7.548809807	1.466185712	1.146028738	CORE	29	O	O	0.0000	29
O	0.753788791	6.069689189	3.345588663	CORE	30	O	O	0.0000	30
O	1.580397844	7.739741559	7.837011978	CORE	31	O	O	0.0000	31
O	8.375398655	3.136294252	5.637456488	CORE	32	O	O	0.0000	32
N	6.622692806	2.354368573	8.971320554	CORE	33	N	N	0.0000	33
N	3.333238797	6.957926874	4.503210328	CORE	34	N	N	0.0000	34
N	2.506566158	6.851558778	0.011733931	CORE	35	N	N	0.0000	35
N	5.796017894	2.248080617	4.479947564	CORE	36	N	N	0.0000	36
H	6.656537196	3.032563886	8.226619342	CORE	37	H	H	0.0000	37
H	3.299366490	7.636026803	5.247942028	CORE	38	H	H	0.0000	38
H	2.472715808	6.173402263	0.756421088	CORE	39	H	H	0.0000	39
H	5.829839317	1.569915573	3.735132215	CORE	40	H	H	0.0000	40
H	5.846292644	2.018462269	0.375131495	CORE	41	H	H	0.0000	41
H	2.456329958	6.621948332	4.116486370	CORE	42	H	H	0.0000	42
H	3.282943561	7.187485363	8.607882482	CORE	43	H	H	0.0000	43
H	6.672891675	2.584055133	4.866564795	CORE	44	H	H	0.0000	44
C	3.797751384	1.885650138	0.469586469	CORE	45	C	C	0.0000	45
C	4.504908045	6.489182677	4.022009898	CORE	46	C	C	0.0000	46
C	5.331532978	7.320346368	8.513411632	CORE	47	C	C	0.0000	47
C	4.624357836	2.716773365	4.960997119	CORE	48	C	C	0.0000	48
N	4.307704920	2.346398129	8.863389559	CORE	49	N	N	0.0000	49
N	5.648161369	6.949878219	4.611219749	CORE	50	N	N	0.0000	50
N	4.821519041	6.859593822	0.119692580	CORE	51	N	N	0.0000	51
N	3.481022478	2.256112054	4.371923657	CORE	52	N	N	0.0000	52
H	4.352719054	2.755473931	7.938607665	CORE	53	H	H	0.0000	53
H	5.603179314	7.358878538	5.536030895	CORE	54	H	H	0.0000	54
H	4.776530235	6.450500944	1.044478199	CORE	55	H	H	0.0000	55
H	3.526088938	1.847030122	3.447082006	CORE	56	H	H	0.0000	56
H	1.785246938	1.894776092	0.146487727	CORE	57	H	H	0.0000	57
H	6.517355930	6.498195337	4.345247654	CORE	58	H	H	0.0000	58
H	7.344006979	7.311227206	8.836618597	CORE	59	H	H	0.0000	59
H	2.611876137	2.707782706	4.637840388	CORE	60	H	H	0.0000	60
O	3.755764148	1.096942297	1.458834324	CORE	61	O	O	0.0000	61
O	4.546933886	5.700443670	3.032758091	CORE	62	O	O	0.0000	62



O	5.373524664	8.109001369	7.524226621 CORE	63	O	O	0.0000	63
O	4.582337719	3.505619394	5.950278115 CORE	64	O	O	0.0000	64

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