Supporting Information

For

Determination of the Cu(III)-OH Bond Distance by Resonance Raman Spectroscopy using a Normalized Version of Badger's Rule

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Cross Validation. A 5-fold cross validation method was used to ensure the predictive power of the Badger's fit in Figure 3c.¹ All the data (bond length and normalized frequency, v_{μ}) from Tables S3-S7 was collected into one master table. The data was randomly sorted into 5 equal groups. One group was selected as the 'test set' while the remaining four groups were used as the 'training set' where this data was fit using the Badger's rule equation (eq. 4). The obtained fitting equation was used to predict the bond length of the 'test set' data. This process was repeated so that each of the five groups became the 'test set'. Of the five 'training sets', the average value of C_{ij} was 182.3 ± 0.5 , while d_{ij} was 0.257 ± 0.002 . The root mean squared error (RMSE) was calculated for all data when it was designated the 'test set'. The obtained RMSE was 0.03 Å, which is the exact same value as calculated for the fitting of the entire data set, indicating that this correlation has excellent predictive power.

Bond Valence Sum Analysis

Bond Valence =
$$e^{((R - R)/B)}$$
 (S1)

Bond Valence Sum (BVS) equation used in Table 3, where R is the bond distance and R_0 and B are parameters specific to the bond of interest. The calculated bond valences are summed together to determine oxidation state of the metal center.²

Atomic Pair	Reduced Mass (µ)
N-N	7.0
0-0	8.0
S-S	16.0
Cr-O	12.2
Mn-O	12.4
Mn-N	11.2
Fe-O	12.4
Fe-N	11.2
Cu-O	12.8

Table S1. Calculated reduced masses used in this work (from unitless relative atomic masses).



Figure S1. Frozen solution rR spectrum of $1({}^{16}O)$ (red) and $1({}^{18}O)$ (black) in CH₂Cl₂ at 77 K using 515 nm excitation. Asterisk indicates solvent peak.



Figure S2. Frozen solution rR spectrum of **2** (black) in DFB at 77 K using 514.5 nm excitation. Asterisk indicates solvent peak.



Figure S3. Frozen solution rR spectrum of **3** (black) in DFB at 77 K using 514.5 nm excitation. Asterisk indicates solvent peak.



Figure S4. Frozen solution rR spectrum of **1** (red line) in DFB at 77 K using 515 nm excitation. Asterisk indicates solvent peak. DFT predicted rR spectrum (black bars), normalized to the 633 cm⁻¹ peak (mPWPW/TZVP).



Figure S5. Frozen solution rR spectrum of **2** (black line) in DFB at 77 K using 514.5 nm excitation. Asterisk indicates solvent peak. DFT predicted rR spectrum (blue bars), normalized to the 628 cm⁻¹ peak (*m*PWPW/TZVP).



Figure S6. Frozen solution rR spectrum of **3** (blue line) in DFB at 77 K using 514.5 nm excitation. Asterisk indicates solvent peak. DFT predicted rR spectrum (black bars), normalized to the 628 cm⁻¹ peak (mPWPW/TZVP).

Structure	CSD RefCode	XRD Cu-O (Å)	DFT Calc. Cu-O (Å)	DFT Calc. v _{Cu-O} (cm ⁻¹)	Normalized Frequency, ν _μ (cm ⁻¹)
	AKONAQ ⁴	1.804(2)	1.805	605	47
	GOWCUQ⁵	1.849(5)	1.925	481	38
Me,ti OH CIQ	LEFXOJ ⁶	1.875(2)	1.878	514	40
	PUXWAG ⁷	1.895(4)	1.949	446	35
	UKARON ⁸	1.887(1)	1.943	456	36
	YETNIU02 ⁹	1.878(2)	1.924	457	36

Table S2. Structures mined from the Cambridge Structural Database $(CSD)^3$, and DFT calculated values using *m*PWPW/TZVP used to construct Figure 3.

Structure	DFT Calc. Cu-O (Å)	DFT Calc. v _{Cu-O} (cm ⁻¹)	Normalized Frequency, v _µ (cm ⁻¹)
	1.816	601	47
OH OH O O O O O O O O O O	1.869	516	40
	1.795	591	46
	1.815	599	47
$O_2 N \xrightarrow{OH} OH \xrightarrow{N \xrightarrow{O} Cu^{ } - N} O$	1.813	598	47

Table S3. DFT Calculated values using *m*PWPW/TZVP used to construct Figure 3.

Bond Type	Core	DFT Calc. Distance (Å)	DFT Calc. v (cm ⁻¹)	Normalized Frequency, ν _μ (cm ⁻¹)	Ref
Fe-O(H)	Fe-O	1.627	852	69	10
	Fe-O	1.634	836	67	
	Fe-O	1.648	804	65	
	Fe-O	1.648	793	64	
	Fe-O	1.652	792	64	
	Fe-O	1.652	785	63	
	Fe-O	1.669	754	61	
	Fe-OH	1.762	616	50	
	Fe-OH	1.779	601	48	
	Fe-OH	1.812	594	48	
	Fe-OH	1.814	588	47	
	Fe-OH	1.813	565	45	
	Fe-OH	1.850	546	44	
	Fe-OH	1.852	536	43	
	Fe-OH	1.893	494	40	
	Fe-OH	1.905	488	39	
	Fe-OH	1.920	462	37	
	Fe-O	1.671	783	63	
	Fe-O	1.652	792	64	
	Fe-O	1.680	749	60	
	Fe-O	1.817	589	47	
	Fe-O	1.806	610	49	
	Fe-O	1.650	819	66	
	Fe-O	1.770	666	54	
	Fe-OH	1.891	497	40	
	Fe-OH	1.869	526	42	
	Fe-OH	1.884	486	39	
	Fe-OH	1.925	450	36	
	Fe-OH	1.913	477	38	
	Fe-OH	1.936	462	37	
	Fe-OH	1.768	657	53	
	Fe-OH	1.838	579	47	
0-0	O_2^+	1.122	1946	243	11
	$\overline{O_2(T)}$	1.220	1550	194	
	Cu-O ₂	1.329	1124	141	
	$Cu-O_2$	1.322	1111	139	
	$Cr-O_2$	1.339	1086	136	
	NaO ₂	1.369	1087	136	
	Co-O ₂	1 380	987	123	

Table S4. Bond distances and frequencies from DFT geometry optimized structures for Fe-O(H) (B3LYP/6-311G) and O-O (*m*PWPW91/DVZP-TZVP) used to construct Figure 3.

Cr-O ₂	1.361	1034	129	
O_2^-	1.363	1097	137	
LiO ₂	1.364	1097	137	
Mn-O ₂	1.377	1009	126	
NiO ₂	1.382	982	123	
Cu-O ₂	1.376	1013	127	
Cu-O ₂	1.358	1041	130	
Pd-O ₂	1.400	941	118	
Mn-O ₂	1.430	937	117	
H_2O_2	1.471	892	112	
Al-O ₂	1.691	543	68	

Bond type	Core	EXAFS/XRD (Å)	Exp. v (cm ⁻¹)	Normalized Frequency, ν _μ (cm ⁻¹)	Ref
Cu-O	Cu-(μ - η^{1} : η^{2} -O ₂)-Fe	1.870	515	40	12
	$Cu_2 - (\mu - O)_2$	1.810	609	48	13
	Cu-O-O-Cu	1.852	561	44	14
	Cu-OOR	1.887	518	41	15
	Cu ₂ -(µ-O) ₂	1.814	610	48	16
	$Cu_2-(\mu-O)_2$	1.828	600	47	17
	$Cu_2-(\mu-O)_2$	1.806	612	48	18
	Cu-(µ-O) ₂	1.840	554	43	19
	Cu-OOR	1.810	652	51	20
	Cu-OR	1.8324	592	46	21
Mn-O	Mn-O	1.560	979	79	22
	Mn-O	1.550	975	79	22
	Mn-O	1.771	700	56	23
	Mn-O	1.760	737	59	23
	Mn-O	1.680	746	60	23
	Mn-O	1.555	979	79	24
Fe-O	Fe-O	1.813	671	54	23
	Fe-O	1.680	799	64	23
	Fe-O	1.640	824	66	25
	Fe-O	1.640	839	67	25
	$Fe_2-(\mu-O)_2$	1.79	673	54	26
	$Fe_2-(\mu-O)_2$	1.78	674	54	27
	Fe-O	1.667	826	66	28
	Fe-O-Fe	1.77	850, 381	49	29
	Fe-O-Fe	1.76	885, 363	50	
	Fe-O-Fe	1.795	838, 409	50	
	Fe-O-Fe	1.77	860, 403	51	
	Fe-O-Fe	1.76	870, 458	53	
	Fe-O-Fe	1.79	827, 395	49	
	Fe-O-Fe	1.78	795, 425	49	
	Fe-O-Fe	1.765	846, 422	51	
	Fe-O-Fe	1.765	850, 425	51	
	Fe-O-Fe	1.79	763, 494	51	
	Fe-O-Fe	1.79	772, 497	51	
	Fe-O-Fe	1.785	770, 499	51	
	Fe-O-Fe	1.80	778, 454	50	
	Fe-O-Fe	1.78	749, 540	52	
	Fe-O-Fe	1.80	745, 537	52	
	Fe-O-Fe	1.785	727, 537	51	

Table S5. Bond distances from EXAFS/XRD and experimental frequencies for the data set used to construct Figure 3.

	Fe-O-Fe	1.79	725, 525	50	
	Fe-O-Fe	1.785	749, 528	51	
	Fe-O-Fe	1.765	768, 507	51	
	Fe-O-Fe	1.78	756, 493	50	
Fe-N	Fe-N	1.53	1034	92	30
	Fe-N	1.526	1008	90	31
	Fe-N-Fe	1.54	918	82	32
Mn-N	Mn-N	1.512	1050	94	33
Cr-O	CrO_2Cl_2	1.580	984	80	34
	CrO_4^{2-}	1.660	847	69	
	$Cr_{2}O_{7}^{2}$	1.630	904	74	
	$Cr_{3}O_{10}^{2}$	1.598	956	78	
	$Cr_4O_{13}^{2-}$	1.587	963	79	
	K_2CrO_4	1.650	874	71	
	$K_2Cr_2O_7$	1.630	902	74	
	$K_2Cr_3O_{10}$	1.593	945	77	
	$K_2Cr_4O_{10}$	1.587	957	78	
	CrO ₃	1.578	975	80	
N-N		1.115	2109	301	35 ^a
		1.113	2031	290	
		1.07	2127	304	
		1.144	2040	291	
		1.08	2116	302	
		1.09	2053	293	
		1.104	2124	303	
		1.11	2038	291	
		1.106	2086	298	
		1.107	2138	305	
		1.107	1979	283	
		1.105	2090	298	
		1.085	2028	290	
		1.12	2004	286	
		1.119	1976	282	
		1.13	2033	290	
		1.106	2041	291	
		1.107	2111	301	
		1.113	2148	307	
		1.095	2153	307	
		1.112	2072	296	
		1.117	1959	280	
		1.136	2043	292	
		1.054	2143	306	
		1.085	1934	276	
		1.099	2142	306	

		1.12	1897	271	
		1.087	2010	287	
		1.102	2090	298	
		1.065	2008	287	
		1.123	2063	295	
		1.094	2122	303	
		1.18	1719	245	
		1.167	1818	260	
		1.237	1414	202	
		1.239	1418	202	
		1.096	2142	306	
		1.235	1548	221	
		1.144	2024	289	
		1.246	1370	196	
		1.286	1270	181	
		1.208	1685	241	
		1.166	1760	251	
		1.2145	1630	233	
		1.239	1503	215	
		1.265	1349	193	
		1.124	2005	286	
		1.132	2007	287	
		1.131	2042	292	
		1.136	1939	277	
		1.151	1770	253	
		1.18	1810	258	
		1.192	1778	254	
		1.215	1625	232	
		1.238	1583	226	
		1.241	1589	227	
		1.12	2164	309	
		1.211	1598	228	
		1.22	1599	228	
		1.185	1696	242	
		1.1	2359	337	
		1.25	1556	222	
		1.45	885	126	
O-0	O_2^+	1.123	1858	232	11
	$O_2(T)$	1.208	1549	194	
	$O_2(S)$	1.216	1484	186	
	Sm-O ₂	1.319	1124	141	
	Cr-O ₂	1.325	1104	138	
	Cr-O ₂	1.327	1072	134	
	NaO_2	1.33	1094	137	

	Co-O ₂	1.355	961	120	
	Cu-O ₂	1.39	961	120	
	Cu-O ₂	1.392	974	122	
	Pd-O ₂	1.411	891	111	
	Co-O ₂	1.429	890	111	
	Mn-O ₂	1.43	892	112	
	H_2O_2	1.453	880	110	
	Co-O ₂	1.457	861	108	
_		1.302	1123	140	35 ^{<i>a</i>}
		1.347	971	121	
		1.432	920	115	
		1.438	924	116	
		1.424	910	114	
		1.432	931	116	
		1.436	884	111	
		1.428	892	112	
		1.488	868	109	
		1.438	882	110	
		1.46	890	111	
		1.445	873	109	
		1.461	893	112	
		1.44	968	121	
		1.21	1580	198	
		1.33	1098	137	
		1.49	877	110	
	Cu_2 - S_2	2.214	442	28	36
	Cu_2-S_2	2.2007	443	28	
	Cu_2-S_2	2.1265	454	28	
	Cu_2-S_2	2.2138	424	26	
	Cu_2-S_2	2.2007	435	27	
	Cu_2-S_2	2.2013	441	28	
	Cu_2-S_2	2.2060	428	27	
	Cu_2-S_2	2.2130	432	27	
	Cu_2-S_2	2.165	440	27	
	Cu_2 - S_2	2.1691	443	28	
	Cu_2 - S_2	2.073	500	31	
	Cu_2 - S_2	2.044	499	31	
	Ir_2-S_2	1.9500	613	38	
	Mo-S ₂	2.07	528	33	
	Mo-S ₂	2.01	530	33	
	Nb-S ₂	2.02	558	35	
	Mo_2-S_2	2.01	540	34	
	$Mo_2-S_2(S_2)_2$	2.08	510	32	
	$Mo_4-(S_2)_5$	2.04	536	33	

S-S

$Mo_4-(S_2)_5$	2.05	550	34	
Ru_2-S_2	2.01	514	32	
Fe_2-S_2	2.02	507	32	
$Mo_4-(S_2)_6$	2.08	480	30	
$Fe_4-S_2(S_2)_2$	2.04	503	31	
$Fe_4-S_2(S_2)_2$	2.05	478	30	
$Mo_2 - (S_2)_6$	2.04	550	34	
$Mo_2 - (S_2)_2$	1.98	561	35	
Nb_2-S_2	2.03	588	37	
$Mo_3-(S_2)_6$	2.02	545	34	
$Mo_3-(S_2)_3$	2.03	562	35	
Fe_2-S_2	2.01	555	35	
Mo_2-S_2	2.04	518	32	
Mo_2-S_2	2.00	520	32	
S_2	1.892	718	45	

^{*a*} Cores not identified by reference 35.

Table S6. Enzyme intermediates with experimental determination of both bond length and stretching frequency used to construct Figure 3.

Enzyme (Intermediate)	Core	Exp. Bond Length (Å) ^a	Exp. v (cm ⁻¹)	Normalized Frequency, ν _μ (cm ⁻¹)	Ref.
HRP-(I)	Fe-O	1.673	790	64	37, 38
HRP-(II)	Fe-O	1.704	789	63	38, 39
CPO-(I)	Fe-O	1.65	790	64	40, 41
CPO-(II)	Fe-O	1.82	565	45	42, 38
TauD-(J)	Fe-O	1.62	821	66	43, 44
Mb-(II)	Fe-O	1.658	805	65	45
sMMO-(Q)	Fe ₂ -O ₂	1.77	690	55	46, 47
oxyHc	O-O	1.51	742	93	48, 49

(a) Determined by EXAFS/XRD and estimated standard deviations indicated in parentheses. Abbreviations: CPO is chloroperoxidase, HRP is horse-radish peroxidase, Mb is myoglobin, oxyHc is oxyhemocyanin, sMMO is soluble methane monooxygenase, TauD is alphaketoglutarate-dependent taurine dioxygenase.

Note for Figure S7. The simple correlation we have discovered also seems to break down upon analysis of diatomic molecules in the gas phase (Figure S7). In addition to the well-behaved line already described, four new trend lines (or striations) appear (Figure S7c). Any diatomics featuring -H or $-^{2}H$ bonds form striations above the Badger's rule trend line in Figure

3c ($v_{\mu} < \sim 300 \text{ cm}^{-1}$), while many metal-metal diatomics fall below the line ($v_{\mu} > \sim 30 \text{ cm}^{-1}$). It is unclear at this time why these significant deviations are observed for these simple diatomic species in the gas phase, however, our Badger's rule correlation still retains predictive power within the limitations we have outlined.



Figure S7. Plots featuring diatomic data⁵⁰ (red) with the prior data set (from Figure 3. black) with bond length vs. frequency, v (a); force constant, *k* (b); and normalized frequency, v_{μ} (c). Graph (d) is a zoom-in of graph (c).

DFT Geometry Optimized Structures

Table S7. Cartesian coo	rdinates (Å) for [1]	7
Atom X	Y 0.02447452057462	<u> </u>
Cu -0.055504114/5855	0.0244/45305/465	-0.00008232207279
H -0.62326362263789	0.49626546187142	2 22948007179556
N 1.13204138775386	-0.29034894785891	-1.53161797885440
C 2.45370567753487	-0.13968637935263	-1.37140464839149
C 3.32069249318627	-0.36957401345754	-2.44086535182861
H 4.39017640034538	-0.24089187733869	-2.28319692270433
C 2.77216060730430	-0.75495470406743	-3.66934702443678
H 3.42657569663352	-0.94064157766068	-4.52238036562030
C 1.38/61152483421	-0.90110179757954	-3.80/63349645424
H 0.9118524/50/011 C 0.57081200780818	-1.195239/8128340	-4./4104300330399
C -0.93205806920179	-0.76039726993359	-2 68453979828660
N -1.43949611087132	-0.47762544292454	-1.46363605081393
C -2.84042737275677	-0.48388178834145	-1.27213881300093
C -3.62930042672373	0.61458758436079	-1.70256133175268
C -5.00945299461565	0.58928812579854	-1.47208567747141
Н -5.62094272440383	1.42957933503369	-1.80730341876371
C -5.61701101021682	-0.48164460/36260	-0.81831610421143
H -0.094/8009892989	-0.48204034013/13	-0.04034134408/00
H -5 30507305766381	-1.3480/398938232	-0.38528017095514
C -3 44979706053423	-1 57063132921497	-0 59548725134600
C -2.62801388405215	-2.75197979357028	-0.10045732200246
Н -1.58771058469559	-2.55611314176890	-0.39273410190212
C -2.66160750208567	-2.84968500129292	1.43495191084783
Н -2.30690848828112	-1.90619513483703	1.87182751571673
Н -2.01355057123920	-3.66885659383658	1.78329460173320
H -3.68043864044971	-3.05070740477847	1.80024609841668
U -3.03966/24013930	-4.00980774392303	-0./08/403/230104
Н -5.00507557109192	-3.99400938143301	-1.80297090892710
H -2 40957282464077	-4 89691705963340	-0 44532626690098
C -3.00687641884899	1.81347476208992	-2.40493341268323
Н -1.92010046167479	1.65940156435011	-2.39849499036727
C -3.28552560349141	3.12609941826578	-1.65090537997335
Н -2.94396212342878	3.05904274584308	-0.61003727926974
H -4.35918141337627	3.3654/890962423	-1.63985949049221
H -2./0324454245520 C -3.45522260188340	3.900199080/0213	-2.1331081131/440
H -3 21648587813325	0.96691166647587	-4 40115142850019
Н -2.94712161118235	2.73067382168054	-4.38869136290517
H -4.53973426651909	2.07294490471384	-3.94987213699983
O -1.53096458867815	-1.07394009875767	-3.73419560322151
C 2.88610243264775	0.28493129296523	0.01716600202575
O 4.09784948730919	0.44723310868167	0.26689496820147
N 1.82240200152625	0.44112961586731	0.83884190642226
C 1.75272620227005	0.82493930330976	2.184/3883421234
C 1 89867795503842	2 52187028676281	3 91968906878611
H 1 69832508113476	3 55159702873161	4 22198739342164
C 2.29484466995660	1.59071984761579	4.87827699159865
Н 2.40517903477574	1.88793256698286	5.92242553427948
C 2.54409407601842	0.27450604411627	4.49144530204329
H 2.84929614348984	-0.45548751050579	5.24369229318629
C 2.40757999802684	-0.13305121136618	3.15914946280984
C 2.68008113133641	-1.581900068/9240	2.//90/950142/28
П 2.40020090751185	-1.09031480388390	2 0102305/380/01
H 4 77820958856829	-1 23161306947044	2.30534565181861
H 4 37197172417268	-2 94860743381740	2 56716543486305
H 4.50829493414714	-1.84778277377537	3.95715435433682
C 1.80640547292991	-2.56374228878907	3.57966307785418
H 1.97628112133100	-3.59520291125170	3.23677479414215
H 0.74019697391308	-2.33425409640222	3.45473209041038
H 2.03800265749086	-2.52995969119422	4.65445275848397
C 1.54169577481600	5.21529252056992	1.54958501486718
C 2 43283200765055	4 28683585648051	1 38070880137744
Н 3.39373194354607	3.83010430747228	1.10977254386807
Н 2.57946778601868	4.85619447954472	2.31094410695255
H 2.15409907832606	5.00103405975714	0.59136462443265
C -0.02421569003729	3.83829817456512	1.88137543467897
Н -0.79840531025921	3.06161526606336	1.93672798998838
н -0.31670209582870	4.55732925929260	1.10172097563640
н -0.00106184258485	4.5//9044/188470	2.84009928969222
Table S8. Cartesian coo	rdinates (Å) for 1	_

A	tom	X	Y	Z
C	1 0.052	43399893838	0.05556684315186	-0.15420836659202
0	-1.102	773608645592	0.37442792395016	1.20493217392966
Η	-0.594	432911949861	0.70670248029755	1.96587651365100
Ν	1.178	53098245986	-0.27674827222176	-1.61935500368437
С	2.485	20711517521	-0.05321517437184	-1.45974028873672
С	3.352	22845778104	-0.27820123175862	-2.52693145254756
Η	4.416	60275266467	-0.09355776643995	-2.39132063370805
С	2.809	18046803375	-0.73435288998520	-3.73497945684745
Η	3.464	80376949294	-0.91923713569107	-4.58566652200514

C	1 42104222460462	0.05412560677207	2 96092105295772
L L	0.072944(0101222	-0.93413300077397 -	4.782((244712(22
н	0.9/284469191555	-1.30/295888/09/9 -	4./8200244/13033
С	0.622/66585/5/0/	-0.70844398852012 -	2.75324781189920
С	-0.87567570211106	-0.87367551062645	-2.66399424650217
Ν	-1.33298748347703	-0.54346519239849	-1.41543871734446
С	-2.69823082092689	-0.60730957684609	-1.07753367031616
С	-3.53155240086787	0.52130640870221 -	1.30565702747946
Ċ	-4 88778441393209	0.41657647804913 -	0 98721493408356
н	-5 54765673408706	1 26479948900765	1 17104245225409
C	5 41160014545180	0.75227056028844	0 42622700745745
п	-3.41100014343189	0.01006072002610	0.10000000754115
п	-0.47230300230810	-0.810808/2023019	-0.19088828734113
C	-4.5/905//0994255	-1.84381994307721	-0.19052837738974
Н	-4.99950829775840	-2.74822741092220	0.24999945358821
С	-3.21628980848386	-1.79562607155500	-0.49287090242695
С	-2.33596732366619	-3.00821507807684	-0.23924734670380
Η	-1.29363007055128	-2.68567641104874	-0.36797502297195
С	-2.47703896660912	-3.54077569866976	1.19630850860292
Н	-2 29485608214632	-2 74633208635767	1 93016297561808
н	-1 75472604547134	-4 34977067913413	1 37313957747624
н	-3 47929732639983	-3 95233749669327	1 38014526933531
C	-2 61373638097298	-4 11404243325416	1 27667541771126
н	-2.48143086406863	-3 742824295225410	-2 30107005122242
ц	2.40145000400005	4 48670067455080	1 19292000170750
11	1 02227407074016	4.06285820100215	1 12406284700862
С	-1.9555/40/9/4910	-4.90363629190313	-1.12400364/90802
U U	-2.99238703038331	1.60/05554654154 -	1.91126/6964/051
П	-1.90135/02821220	1./02082/9452859 -	1.98545106152764
U U	-3.2/88203212029/	3.02555462521564 -	1.01500157615402
н	-2.88530043126104	2.809/3853008202 -	0.0055/64844/022
Н	-4.356/6842153662	3.22423032855431 -	0.935340/1229390
Н	-2.8089/1/464/956	3.92512301235525 -	1.4369/643659/42
С	-3.53725736119797	2.01/322281/920/ -	3.33752876166125
Н	-3.30989533526082	1.15714789671111 -	3.98002325829942
Н	-3.09318165027757	2.91565411708061 -	3.78946127039562
Н	-4.62829440967379	2.15273482528903 -	3.32471455436712
0	-1.54120635147597	-1.26209366426295	-3.62682567692399
С	2.84858095633635	0.43379129686137 -0).07695166754486
0	4.01389005851469	0.68494797757109 0.	.23806255890978
Ν	1.73628651694074	0.53912581827824 0.	.71726889521624
С	1.83962267261903	0.97241972402025 2.	.06403828486033
С	1.79984950643355	2.36081211897124 2.	.36188680444474
С	1.88522961400533	2.75189274807695 3.	70253822004046
Н	1.86443334019581	3.81344455973937 3.	.95320675750296
С	2 00052978376018	1 81154131413834 4	72406175596681
н	2 06592745782710	2 13991020469483 5	76179341880155
C	2.02882952801421	0.45137762940595 4	42011045447942
н	2 11701713/70552	-0.27501101000636 5	5 22716472921232
C	1 0//1/878535202	0.00202341281614 3	00773108331417
č	2.00707456501286	1 49646926119440 3	070768517740815
п	1 74206007405220	1 61220024750255 1	
П	1./429090/403550	-1.01526924756255 1	07000781(50000
U U	3.440/03/10/0338	-2.02139437471767 2	2771578(0(7017
н	4.15985511278509	-1.4551/284580/46 2	2.5//15/8090/91/
н	3.49813/3962/842	-3.0/885515510/46 2	2.68468411397579
Н	3.75059695298790	-1.95050783268270 4	1.03226852904905
С	0.99392226507581	-2.29736009381390 3	3.61724604272510
Н	1.00711027196690	-3.35053156636913 3	3.30402010052717
Н	-0.02545304492748	-1.91436745605959	3.48015883344722
Η	1.22705763394973	-2.27042149835598 4	4.69086839856505
С	1.69493389557067	3.41469433365941 1.	26977091584876
Н	1.57667064443947	2.88585196725161 0.	.31467263439903
С	2.98640191254615	4.24999009828886 1.	18216261155353
Н	3.86157985019334	3.60768350507698 1.	.02422450994120
Н	3.14901928910833	4.82750274642393 2.	.10353686096631
Н	2.92505352777230	4.96403726591277 0.	.34836684306991
С	0.45780936677044	4.31110104971705 1	45267166877836
Ĥ	-0.46258714230172	3.71373233574339 1	49258060323591
н	0 37027953836114	5 01643495981293 0	61395354653441
Н	0.51879092349886	4.90153843897864 2	37721599324427
T٤	able S9. Cartesian co	ordinates (Å) for MeLCu	ин-ОН
At	om X	Y	Z
С	u 0.00817935040076	-0.06454268629597	0.01620223080041
0	1 14402427228169	0 15070//8030551	1 40145116713953

Cu 0.00817935040076	-0.06454268629597	0.01620223080041
O -1.14403437328168	0.15979448039551	1.40145116713953
Н -0.64275980218238	0.49812479502953	2.16767419634998
N 1.11944172387145	-0.28038198372650	-1.48109264357391
C 2.42031377943720	-0.02135537570799	-1.32901029296226
C 3.27681718584408	-0.15975304066222	-2.41914056090415
Н 4.33644260498963	0.05296289087848	-2.28850825863576
C 2.72950315239592	-0.56741336035274	-3.64236779555116
Н 3.37696616804660	-0.68356726825855	-4.51120476580289
C 1.35726220543300	-0.82035992384245	-3.76111259389468
Н 0.89269757302322	-1.12957021028543	-4.69583325253738
C 0.55902455832218	-0.66445058858994	-2.62946062327811
C -0.93575344956130	-0.85816508590098	-2.53587699662668
N -1.38118048339079	-0.64444970738028	-1.25719126244470
C -2.74320473999677	-0.68343800431905	-0.91905730561762
C -3.59984784372472	0.38120834785126	-1.30106823721273
C -4.94813018483548	0.30798672795398	-0.94553089535581
H -5.61964508408472	1.11496243190115	-1.24159584030910
C -5.44138119072661	-0.77471765415754	-0.21456514730560
H -6.49675115894451	-0.81163596321117	0.05671395486215
C -4.58622463336339	-1.80697065154795	0.17274576974769
Н -4.97463165181967	-2.64918367647389	0.74668209080838
C -3.23006124813326	-1.77890082026119	-0.16058885617773

C -2.30705893330362	-2.88363510588354 0.26884840905081
H -1.56723764408257	-2.49930509750571 0.98554159193293
H -2.86634438343558	-3.69425828378283 0.75073881147943
H -1.75425359336476	-3.30251631290311 -0.58300511996910
C -3.07468916644637	1.54906969587906 -2.08755566844004
H -2.19812647181032	1.99685311840840 -1.59863173359439
H -2.76575589550559	1.23561961192856 -3.09532981072604
H -3.84275964582321	2.32421588677930 -2.19241999053067
O -1.60774314283427	-1.17751057044069 -3.51924364947046
C 2.78816256140028	0.42099860593143 0.06792903683646
O 3.9441444634405	0.72556319636963 0.36965411634738
N 1.69131671378842	0.41982688424007 0.89084162527449
C 1.78728377653346	0.84134421671184 2.23790366969484
C 1.82348819482016	2.22408133325123 2.54416777706084
C 1.88644956343255	2.60489526667230 3.88854715531616
Н 1.92092810787852	3.66638272378062 4.13721650985733
C 1.90265805916580	1.65105368605384 4.90681756987921
H 1.94812329380971	1.96786220946158 5.94890360487544
C 1.85876653799778	0.29235548157811 4.59270900895397
Н 1.87524756276896	-0.45183685924326 5.38989639869021
C 1.79733401313706	-0.13705836407777 3.26272739196408
C 1.76052759539452	-1.60285814205836 2.92482971978385
H 0.83210439260226	-1.86322067165206 2.39601377346327
Н 2.59554450464452	-1.88216291173506 2.26776686506041
Н 1.81902745461535	-2.21303960244653 3.83369413496129
C 1.81406514330223	3.25563569180452 1.45001109258153
H 0.97389563391374	3.09917188566205 0.75901641704344
Н 1.73278551904470	4.26592668821013 1.86758169478618
Н 2.73884502429347	3.20400803597016 0.85752066631930
Table S10. Cartesian co	ordinates (A) for 2
Atom X	<u>Y</u> <u>Z</u>
Cu 0.111/6989442788	0.02808209097871 -0.17239018786638
U -1.00920519224/60	0.52415570105905 1.17541247551895
N 1 25011848007658	0.00595195824948 1.94/15150055099
C 2 55478242102506	-0.28781403771990 -1.05313029480775
C 2.33478242103500	0.27770542250550 2.52622236267122
H 4 49373509386529	-0.00100/88252201 -2.381771007507/0
C 2 80776665546602	-0.72707626092475 -3.74153035429905
Н 2 56000258427222	0.00420414802112 4.58842062112725
C 1 52102788008082	0.04066477076712 2.87012200022021
H 1 07105467204662	1 20777628210200 4 80606204140240
C 0 70422277701502	-1.29777028519299 -4.80090504149549
C 0.70422277791392	0.9247780422459 2.60616965902497
N 1 25722651841004	0.56272452100020 1.44600066022485
C = 2.62230967134533	-0.50272455150055 -1.44005500025485
C -3 45447875141417	0.50278214836723 -1.33806142515794
C -4 80836846213211	0.00278214830723 -1.033800142313774
H -5 49034739661152	1 23570112132956 -1 18672041300640
C -5.30532517352415	-0.77162631458463 -0.46891267956084
C -4.49559494350882	-1.87407592315995 -0.21733782271961
H -4.94188961607331	-2.76375349387913 0.22114792755507
C -3.13691264581260	-1.81953100485592 -0.52631279356150
C -2.26093894837085	-3.03577565447123 -0.27822319562602
H -1.21767102830633	-2.71257307220539 -0.39667329548605
C -2.41733957597187	-3.58330962174533 1.14997775770859
H -2.24032385895210	-2.79895078152553 1.89577464731047
Н -1.69837556337301	-4.39565180886959 1.32240749026174
Н -3.42125571582196	-3.99594388809836 1.31958641113606
C -2.53641733121284	-4.12797999106636 -1.33120215326570
H -2.39514734804650	-3.74763850307435 -2.35100983834159
H -3.56/8502/44/68/	-4.49868336218318 -1.24883620602131
H -1.859/9130393931	-4.980/0698304387 -1.1816337/930299
N -6./53654/5091645	-0.8522928/664940 -0.13415/92363641
0 -7.1/3905/6463810	-1.91209/4685/416 0.3449138/035182
C 2 02182840722708	0.14494448505841 -0.55515005952525
C -2.92183849/32/98	1./880859698/269 -1.9489/509925346
H -1.83034284608769	1.688102/1912105 -2.018/39483//641
C -3.21984197808099	3.00923305110435 -1.06077309859029
H -2.82/94932004116	2.80529707871429 -0.04639337395097
H -4.298938095/4805	3.20201282//9/29 -0.9851924//3945/
C 2 46802020562024	1.08421416026280 2.27672222587502
H _3 23710406019911	1.20421410020287 -3.37072223387372
H _3 02068004402067	2 88236/3773053/ _3 83263667383267
H -4 56029886764384	2 11487378854054 -3 36390133807607
Q -1 45996213121847	-1 26542980257450 -3 65921098847689
C 2.90400635769833	0.41611889995122 -0.07585964531746
O 4.06134736344622	0.66988070052652 0.25880664025384
N 1.78231749642650	0.51325010073540 0.71021004035914
C 1.87916531726636	0.93764556372424 2.05860982662596
C 1.84184379060052	2.32655373458052 2.36177930770173
C 1.92442173727975	2.71603626702159 3.70041223879284
Н 1.90770732227363	3.76601634096223 3.98610441442362
C 2.03539852109935	1.75240792652201 4.69586018877330
C 2.06299642736598	0.39170540694371 4.41069955964872
H 2.15085399402333	-0.31523710131230 5.23238856937446
C 1.97942715592716	-0.04122390010673 3.08579285154909
C 2.04008810846613	-1.52937814728564 2.77701079897466
H 1.78183383000344	-1.65105077240605 1.71610603604235
C 3.47207599790022	-2.06619384477313 2.97295165041844
H 4.19773338120940	-1.49924501852913 2.37684871259838

H 3.52734245870171 H 3.77449296021863	2 12242(027002(5	2.67473195332718
H 3.77449296021863	-1 1//4/091/90/05	2.0/4/51/5552/10
H 3.//449296021863	2,000((20(752522	4 00751404122002
C 1 01005477075030	-2.00066206753533	4.02/51494155995
C 1.019954//8/5028	-2.33622715942730	3.59702956257108
H 1 03372926020060	-3 38902563164582	3 28395181465980
II 0.00150706242080	1.05241071278502	2 45467464586260
П 0.00139/90342980	-1.932419/12/8302	5.45407404580200
H 1.24760359973352	-2.30987330001143	4.67152912686407
N 2 12577266070420	2 19118173851848	6 11620552814661
0 2 22072840607458	1 21200122240578	6 08084010260269
0 2.229/384060/458	1.31399133340578	0.98084919200308
O 2.09210666361407	3.40575334326730	6.34394546928446
C 1 74148279915084	3 38969492910977	1 27903216199515
U 1 (201200574227)	2.96905792752199	0.21027225(77442
H 1.03012895/432/0	2.80805/85/52188	0.3193/2236//442
C 3.03199671302479	4.22829619711227	1.20956170282056
H 2 011/2255961920	3 50128145507787	1 05260622006821
11 3.91143233801829	3.39138143397787	1.05509052990851
H 3.1845151/2//115	4.80128658804816	2.13512464281513
H 2.97358686456884	4.94695136600852	0.38010492229703
C 0 50098956780480	1 28083860148400	1 46718068232048
U 0.30078750780480	4.28083803148433	1.40718008252048
H -0.41929262151505	3.682/5021530/58	1.49849949301473
H 0 41617506836328	4 99295262201934	0 63452622130485
H 0 55820054207120	1 86258425020220	2 20642221607727
11 0.55829954207120	4.80338433939220	2.39043221007737
Table S11. Cartesian co	ordinates (Å) for 3	
Atom V	V	7
Atom A	1	<u> </u>
C 0.34287174893289	-0.15480732180605	-0.17101575671476
C -0 40504545060932	-1 15468255064008	-1.05657021048599
NL 0.90200297211752	0.60222226022704	2 10499707929091
-0.0720026/311/53	-0.00333330033/94	-2.17400/0/828081
C -1.84885209587037	-1.28667208032454	-2.97426267974072
C -1 46550139689663	-2 27044430640134	-3 90450566461229
C -2 45700462006265	-2 03/70606507074	-1 61700259720445
C -2.43/70402000200	-2.734/000038/0/4	
C -3.79544754958989	-2.63348527554833	-4.43870572283270
C -4.16348451355568	-1.65532413865432	-3.53061119299260
C 2 21126520759252	0.06526726467095	2 70245210560222
0-3.21130339/38352	-0.9033023040/985	-2.19343218300232
C -3.66526885962690	0.06794631937608	-1.78705556126462
C -4 19211409810886	-0 60647990185965	-0 51813573673587
C -4.17211407010000	-0.00047990103903	-0.51815575075587
H -3.44/40548212522	-1.2//6/206084960	-0.083/9205408891
H -5.08218525738830	-1.20271922664295	-0.73785101673015
H -4 46840261266361	0 14158352857639	0 23088625759166
11 -4.40840201200501	0.141585552857657	0.25088025757100
C -4.69035/344381/9	1.03350300824808	-2.3/081088668/10
H -4.94019296151151	1.81066483560034	-1.64275703804439
H 5 62254600740850	0 52972099626105	2 62552505025202
11 -3.02234009740830	0.32872988020103	-2.033323030333393
H -4.29614160259166	1.510/4826/103/5	-3.26911878579986
H -2.79008844286014	0.66131768161876	-1.50974035865111
Н 5 21200210802816	1 42286165760768	2 20600064657622
Н -3.21390310802810	-1.42280103/09/08	-3.39000904037033
H -4.55319604907588	-3.16349168969568	-5.00534154371041
H -2 17669024093347	-3 70660935101880	-5 32522644575618
C 0.02772617451772	2 69216144267565	4 11885270060404
C -0.02//301/431//3	-2.08510144507505	-4.11883370900494
C 0.21545660628447	-4.08001436689988	-3.54286318374341
H -0 02945704508741	-4 11393730525798	-2 47973671145001
II 1 26164712606228	4 27167056680524	2 67920925500222
П 1.20104/12090238	-4.3/10/930089334	-3.07830833309222
H -0.40199460566706	-4.81982515558609	-4.05895799442365
C 0 36123038910727	-2 64130723139252	-5 59464831416408
11 0 20818468740805	1 64910705109092	6 02271206614428
11 0.20818408740895	-1.04819/95108985	-0.022/1390014428
Н -0.23256717349468	-3.34932375727109	-6.17678678027981
H 1 41038679644964	-2 92544977087591	-5 72061086578487
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H 0 85649406616828	1 28276823297359	2 17539180498689
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H 0.85649406616828 H -0.81086477114327	1.28276823297359 1.74364886943522	2.49311888293812
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909	1.28276823297359 1.74364886943522 3.55015079907541	1.60339215351161 2.17539180498689 2.49311888293812 1.17454399812538
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562	1.60339215351161 2.17539180498689 2.49311888293812 1.17454399812538 0.26878984358189
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562	1.00339215351161 2.17539180498689 2.49311888293812 1.17454399812538 0.26878984358189
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061	1.60339213351161 2.17539180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061 2.97090326248037	1.00339213531161 2.17539180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061 2.97090326248037 3.82507012265584	1.60339215351161 2.17539180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772
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H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610 C -0.90369787736151	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061 2.97090326248037 3.82507012265584 4.39786399708157	1.00339213351161 2.17539180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233
H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610 C -0.90369787736151 C -0.89320025346091	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061 2.97090326248037 3.82507012265584 4.39786399708157 5.15129508541333	1.00339213351161 2.17339180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233 -5.36550095017139
H 0.85649406616828 H -0.81086477114327 H 0.35402540861090 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610 C -0.90369787736151 C -0.89320025346091	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061 2.97090326248037 3.82507012265584 4.39786399708157 5.15129508541333 5.37008927210601	1.00339213351161 2.17339180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233 -5.36550095017139 -6.0649049840763
H 0.85649406616828 H -0.81086477114327 H 0.35402540861090 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610 C -0.90369787736151 C 0.27882549332071	1.28276823297359 1.74364886943522 3.55015079907541 2.83843042251562 3.38539047191061 2.97090326248037 3.82507012265584 4.39786399708157 5.15129508541333 5.37908987219601	1.00339213351161 2.17339180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233 -5.36550095017139 -6.06480483849763
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H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610 C -0.90369787736151 C -0.89320025346091 C 0.27882549323271 C 1.4609201886942 C 1.51155762639393 C 2.85232253342410 C 3.5398980646381 H 2.88189570331774 H 4.44192011583154 H 3.8442825018638 C 3.75202069857295 H 3.23984133726107 H 4.03627274192672 H 4.67113498201136 H 2.6713331337282 H 3.23984133726107 H 0.26533707097457 H -1.81803571924553 C -2.16641261082352 C -2.20982029740649	1.28276823297359 1.7436488643522 3.55015079907541 2.83843042251562 3.8539047191061 2.97090326248037 3.825007012265584 4.39786399708157 5.15129508541333 5.37908987219601 4.08535381895016 4.08535381895016 4.08535381895016 4.08535381895016 4.08535381895016 4.08535381895016 4.73628542747090 5.35068473352115 5.36988990370541 4.34861589126127 2.97734546510630 5.07307562153348 5.97060973917352 5.58132410246506 5.07307562153348	1.00339213351161 2.17339180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233 -5.36550095017139 -6.06480483849763 -5.58706878200811 -4.43594692638253 -3.94995113828231 -4.98111058897662 -5.32066132722001 -4.55522138088112 -5.86036780008063 -3.50489514158120 -2.7634959085647 -4.34944561240807 -3.05682455251017 -3.06493165409172 -6.11652006472750 -6.97340120674780 -5.73001779960078 -3.36507271654298 -2.41188901803308 -2.70154298
$\begin{array}{l} {\rm H}\ 0.85649406616828\\ {\rm H}\ -0.81086477114327\\ {\rm H}\ 0.381002540861009\\ {\rm H}\ -0.97078320139293\\ {\rm C}\ 0.91066895972407\\ {\rm N}\ 0.31505641129037\\ {\rm C}\ 0.30643530815610\\ {\rm C}\ -0.90369787736151\\ {\rm C}\ 0.27882549323271\\ {\rm C}\ 1.46909201896942\\ {\rm C}\ 1.51155762639393\\ {\rm C}\ 2.85232253342410\\ {\rm C}\ 3.53998960463814\\ {\rm H}\ 2.88189570331774\\ {\rm H}\ 4.84192011583154\\ {\rm H}\ 3.84422825018638\\ {\rm C}\ 3.75202069857295\\ {\rm H}\ 3.23984133726107\\ {\rm H}\ 4.03627274192672\\ {\rm H}\ 4.67113313372582\\ {\rm H}\ 2.67133317924553\\ {\rm C}\ 2.16641261082352\\ {\rm C}\ -2.208209746049\\ {\rm H}\ -3.06495674414854\\ \end{array}$	1.28276823297359 1.74364886943522 3.50015079907541 2.83843042251562 2.97090326248037 3.82507012265584 4.39786399708157 5.15129508541333 5.37908987219601 4.86189266965761 4.08535381895016 3.58374900794219 2.69551155787435 1.89133009357564 2.24513600954785 3.26898579016740 5.35068473352115 5.369889519016740 5.35068473352115 5.369889519016740 5.35068473352115 5.36988990370541 2.434861589126127 2.97734546510630 5.070307562153348 5.9706097317352 5.5681342410246606 4.30968637332730 5.50681454859990 5.543072475934111	1.0033213351161 2.17339180498689 2.49311888293812 1.17454399812538 0.26878984358189 1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233 -5.36550095017139 -6.06480483849763 -5.58706878200811 -4.43594692638253 -3.94995113828231 -3.94995113828231 -3.94995113828231 -3.94995113828231 -3.94995113828231 -3.94995113828231 -2.76349540863 -3.50489514158120 -2.7634950085647 -3.30582455251017 -3.06493165409172 -6.11652006472750 -6.97340120674780 -9.7340127966078 -3.35607271654298 -2.41188901803308
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H 0.85649406616828 H -0.81086477114327 H 0.35402540861909 H -0.97078320139293 C 0.91066895972407 N 0.31505641129037 C 0.30643530815610 C -0.90369787736151 C -0.89320025346091 C 0.27882549323271 C 1.4609201886942 C 1.51155762639393 C 2.85232253342410 C 3.5398980646381 H 2.88189570331774 H 4.44192011583154 H 3.8442825018638 C 3.75202069857295 H 3.23984133726107 H 4.03627274192672 H 4.67113498201136 H 2.6713331337282 H 3.6713373282 C -2.16641261082352 C -2.2098209740499 H -3.06495674414854 H -2.31253708270971 H -1.28816140603778	1.28276823297359 1.7436488643522 3.55015079907541 2.83843042251562 3.8539047191061 2.97090326248037 3.825007012265584 4.039786399708157 5.15129508541333 5.37908987219601 4.08535381895016 4.08535381895016 4.08535381895016 4.08535381895016 4.08535381895016 4.08535381895016 4.035385787435 1.89133009357564 2.24513600954785 3.36088473352115 5.360884903070541 4.34861589126127 2.97734546510630 5.07307562153348 5.97060973917352 5.58132410246506 6.43378563581955 5.57847133031588	1.0033213351161 2.17339180498689 2.49311888293812 1.17454399812538 0.26878984358189 -1.47474811060399 -2.61822465057732 -3.75031576350772 -4.19470935982233 -5.36550095017139 -6.06480483849763 -5.58706878200811 -4.43594692638253 -3.94995113828231 -3.94995113828231 -3.94995113828231 -3.94995113828231 -3.94995113828231 -5.86036780008063 -3.50489514158120 -2.76349590085647 -4.34944561240807 -3.05682455251017 -3.06493165409172 -6.97340120674780 -5.73001779960078 -3.36507271654298 -2.41188901803308 -1.73337976115329 -2.98064592376662 -1.8145130007661

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	Н	-1.53105238073584	1.44878444815291	3.99352903872389
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-0.60498544975329	С	-1.01128116413322	-0.48568339246215	-2.62354312666731
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3 11064910708959	н	-3 36657070246012	-0 07349906395287	2.69333679528868
1.41840898987657	н	-5.02637322645597	-0.71307544375795	2.55682597510722
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3 58704085236694	н	-2 56034454196381	0 47651706359139	0 68420710859204
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-3.86441025272389	H	0.413403/3192444	-2.420240/9933924	2.00130055994090
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-5.29029770075644	п	3.09338238447304	-0.3//2/093402/80	-2.200834/814003/
-6 22689891563389	Tal	hle S14. Cartesian co	ordinates (Å) for CSF	Refcode LEEXOJ
-4 99804634356949	Ate	m X	V	Z
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-5.64665119079487	Н	1.61851817661813	-1.63372027116239	-0.88117633210949
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0.51320282959983	С	0.43715684866880	2.85535474590273	-0.61901659032367
-0.01984837673704	C	-0.75627428059621	2.77564728099624	0.33021041052316
1.59089875153340	N	-1.45692186395645	1.459/3576953755	0.23210893646923
0.510/00906/0345	C	-2.2150/172851733	1.154436/8889503	1.48300136983337
0.0330493711/0039	N	-1.3003133204/041	-0.54345324860470	2.300//062401880
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1.93691369505379	й	1.32234820242370	-1.50976246554451	2.38389127102205
	Н	1.26958375999438	0.15845916846517	2.99680607999272
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0.02305962864071	Н	-0.71644894681335	-2.5/6/6/64925895	1.01329232090039

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H -2.23941077904119 -1.65429552858006 1.51752940031028 H -0.59065273016759 1.38831466336859 2.90089195632492

H -1.90746804073571 0.35854069703275 3.46796458846948

H -3.43691285989390	3.38750882139215	-4.87616332945697
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C 2.13546714077085	0.53270053269782	-1.60494380155796
H 2.87976136606791	0.41910873123839	-0.81015569889542
H 2.48225200041546	1.27117332126309	-2.32315541887313
H 2.00454934384745	-0.42230609643418	-2.11387213199627
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Н -1.02526777782519	2.01694811677640	-4.56326565659686
O -0.59157830636173	-2.29184846822032	-0.66342216194869
H 1.20887486576032	-0.65705966655619	0.27092981278441
Table S12. Cartesian co	ordinates (Å) for CSE	Refcode AKONA
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C 1.17105305501517	0.09903661355314	-2.23188984402227
N 2.45156120744893	0.38581778486146	-1.62547336097130
C 3.28467176572128	-0.56954460613435	-1.08852943014619
Cu 3.03527516073791	-2.40968468256640	-0.98816534948781
O 2.71920488530727	-4.18549557871790	-0.93069642354011
H 3.45278492788972	-4.65970022599381	-0.50720602457747
N 4.36072738644905	0.16225484654354	-0.63840045760506
C 4.19690322060907	1.52182618063718	-0.88894260478986
C 2.99453531684109	1.66241623685921	-1.51055639809200
H 2.48050744804891	2.54062554346156	-1.87801303935460
Н 4.94263562079956	2.25240919417146	-0.60498544975329
C 5.51694344975372	-0.40900040366732	0.01402335859296
C 6.61703946694234	-0.80073771074393	-0.77701141209501
C 7.73827470244800	-1.31838912477289	-0.11443283442852
H 8.60333383727055	-1.63458303608560	-0.69739258763233
C 7.76246211774753	-1.44440552123283	1.27237863578338
H 8.64551156947235	-1.84995097211641	1.76692250335837
C 6.65583442243880	-1.06340947646896	2.02721005314955
H 6.67826827069552	-1.18124176298982	3.11064910708959
C 5.50748183293088	-0.53924973022054	1.41840898987657
C 4.29773982664330	-0.17702841326101	2.26941088811076
Н 3.53994730406653	0.26182942808772	1.60737181347295
C 4.63826987634938	0.87353616744581	3.34155773696343
H 5.05993802732918	1./838928/864390	2.89459537225640
H 5.36/18281044196	0.4885/628856112	4.06/84186/822/1
H 3./3402///394069	1.154/0045639337	3.898/2294361398
C 3.6/83851/144989	-1.4406/2052348/6	2.8966/494885283
H 3.40081485902218	-2.169448922/5585	2.12324501816210
H 2.//444080290082	-1.18198520208091	3.40342/8430399/
H 4.381/908//25398	-1.92084439812204	3.38/04085230094
U 5 67572712070611	-0./2002948004813	-2.29/95885089810
C 7 77762206624076	0.10105517420088	2.00238490377290
U 778725024710740	1 11719512007724	-2.84930393429394
П 7.76723924710749	0.10407751520007	2.43043377390490
H 8 74561730741045	-0.36422580817020	-2 61055855600/77
C 6 57780358803200	-2 14125807583044	-2.017558555077477
H 6 51273687469241	-2 08575681363338	-4.00268283666727
H 5 71/70388015700	-2 71318639666643	-2 54034219060461
H 7 49003633247109	-2 69863958441825	-2 65189935920026
C 1 12132462293891	-0 16639646459971	-3 61609106140159
C -0 13652322847154	-0.41579812476331	-4 18125135613478
C -1 29179139884694	-0 40462827187468	-3 40376645109235
C -1.21118660456157	-0.14963640162579	-2.03709435443672
H -2.11944259963384	-0.15843236281181	-1.43447938746349
H -2.25968623191107	-0.60467553832611	-3.86404019963632
H -0.20870437416023	-0.63089841648875	-5.24738106498354
C 2.36819208705874	-0.22482760262689	-4.48836118926721
H 3.22869326093754	0.04999892590053	-3.86441025272389
C 2.30419151019896	0.78115211549353	-5.65182876188614
H 2.15247032096099	1.80715874016824	-5.29029776673844
H 1.48476078911567	0.54624054163180	-6.34501393433862
H 3.24014550483892	0.75716392543737	-6.22689891563389
C 2.61270519925672	-1.65797720040805	-4.99804634356949
H 2.69782095610041	-2.36681947799635	-4.16411477768168
Н 3.54175857241989	-1.70113376941579	-5.58359557416759
H 1.79208300830936	-1.99473166218036	-5.64665119079487
Н 1.11515995407642	0.57623146263643	0.35107495443322
C -0.78838261242999	1.54314278572385	0.51320282959983
н -0.49926343893346	2.45890171868419	-0.01984837673704
н -0.677/2051430529	1./2642500044847	1.59089875153340
н -1.85438929382662	1.36410863387716	0.31676090670345
C -0.31666570855036	-0.933/5736191541	0.85384937170839
п 0.32943/4/195/03	-1.///31/08101521	0.57758875897548
H _0 22658750674162	-1.22043439/339/4	0.04551/58528255
-0.22030/300/4102	0.7704470404040002	1.75071507503579

H -4.30659156115701 4.13653460671759

S13. Cartesian coordinates (Å) for CSI X V Table

		•	
Cu 0.0	03890344189644	0.13967871772783	0.02305962864071
O -1.	02664643080342	0.21809019348651	1.62385514369917
Н -1.	12578967943912	-0.66191099196941	2.02386013540688
N 1.1	7497579812969	0.18564135317540	-1.70010477382030
C 1.1	7587193951630	1.60968432883435	-2.12357777747066

TT 0 7407000010000		
H -2./48/3285813032	2.05127719383235	1.84000886140091
H -2.97960480791973	0.40846025280165	1.23632958843013
C -2.34849230950175	1.40844229936825	-0.96470527164442
C -2 58091431676164	-0.02516320563439	-1 43104926506179
N 1 20176738080570	0.722/2105/200022	1 70812726650776
N -1.301/6/380803/9	-0.72343103489033	-1./0812/20030//0
C -1.48948666547643	-2.19182418159533	-1.69451876764154
Н -0.51731101777333	-2.68112336224075	-1.81090085846735
H -1 91290449769005	-2 50443619449607	-0 73535123778116
Ц 215058510414280	2 51870761671157	2 50822501846670
11 -2.13938319414380	-2.318/0/010/113/	-2.30822391840079
C -0./550/24539196/	-0.32690630572415	-3.02388342688490
H 0.22040100120845	-0.80294609858004	-3.17085477421898
H -0.62188358316243	0.75895817494165	-3.07749606461603
H -1 42558122382948	-0 63757391075747	-3 84441041502387
Ц 2 22797241929217	0.01804278400022	2 21065600185510
11 - 5.25767541626517	-0.010/42/04//025	-2.51905099105519
H -3.1089/63/203896	-0.59544/55465/46	-0.05501550405404
H -1.87326895679625	1.98972816837721	-1.76367964030978
H -3.31380904935269	1.89631748288573	-0.74938687735929
H -0 41703986332010	2 89718316242186	1 36558877505349
Ц 1 45705020780426	2 60260232420106	0 12667520625203
11 -1.45705929789420	3.00200232429190	0.12007329023203
H 0.9462/410/04852	3.82651135980941	-0.4809231/858034
H 0.09681859834344	2.82760826429597	-1.66290391401185
C 2.23953510110546	1.51669198990485	-1.58996375656604
H 2 84202687412779	0.61717152750019	-1 42426747094747
Н 2.01468152620530	2 27662022222601	1 74145050207348
H 2.91408133029339	2.37002922333091	-1./414393020/348
H 1.63595368869023	1.3/984/88530981	-2.49338330153309
C 2.21505348867027	1.90208631185585	0.77771355759208
H 2.77648880104240	0.97774008502325	0.94960149777824
H 2 91847313142393	2 74147437496594	0 63759479390889
Н 1 60117507552010	2 10777874184005	1 66122721011929
11 1.0011/30/332919	2.10///0/4104003	1.00102/01711020
Table 615 Control	andinata- (k) c . corr	Defeed- BUWWY
1 able S15. Cartesian co	orainates (A) for CSI	v Retcode PUXWAG
Atom X	Y	Z
Cu 0 23936846518072	0 20759523255663	0 45602201982434
0 1 43659619420349	-0.80252656972302	1 61518378371441
U 2 2244108004(208	0.204(44999400(2	1.01310370371441
H 2.22441080046308	-0.29464488840063	1.8/324396394233
N -1.00922994004021	1.25818397116959	-0.81088087256295
C -1.14909848803998	0.43916739947278	-2.04169563075596
C -1 33749262508517	-1 02302053468766	-1 70222230564373
N 0.65820005182477	1 45257572462147	0.61505574776802
N -0.038209031824//	-1.4333/3/340314/	-0.01303374770892
C -0./1309080969015	-2.//484859048325	-0.269/9686568/42
N -0.03749157753559	-3.15755400363649	0.83853840805665
C 0.01206063096871	-4.53531945472319	1.31975604323053
C 0 52812516657101	-4 67520417106807	2 77040277101634
C 1 07612247247525	4 16412021444626	2 80012082702010
U 2 (40040115(1510	4 (0228975925772	2.00015005702010
H 2.64004911561519	-4.093288/3823//2	2.19154596450066
H 2.05433765456192	-3.08647448735816	2.68916767478602
H 2 35603976025327	-4.33886908393254	3.90610448917867
11 2.550055770025527		
C 0.49459548215242	-6.17713647333709	3.11112084393937
C 0.49459548215242 H _0 52430533690353	-6.17713647333709	3.11112084393937
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426	-6.17713647333709 -6.58311980133535 6.75660594453612	3.11112084393937 3.03866863727053 2.43735052278088
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426	-6.17713647333709 -6.58311980133535 -6.75669594453612	3.11112084393937 3.03866863727053 2.43735052278988
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426 H 0.84758362703589	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026
H 0.5243053690353 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211 H -0.04453508316695	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -4.04058763708827	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211 H -0.04453508316695 H -0.41010723140260	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005776
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211 H -0.04453508316695 H -0.41010723140260	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -2.83565924478291 4.28565924478291	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211 H -0.04453508316695 H -0.41010723140260 H -1.42255862242347	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291 -4.28500931591561	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430
C 0.49459548215242 H -0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211 H -0.04453508316695 H -0.41010723140260 H -1.42255862242347 H -1.00421853741808	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.3441312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291 -4.28500931591561 -4.95626140449838	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978
$ \begin{array}{c} C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ H & 0.84758362703589 \\ C & 0.39035122027211 \\ H & -0.04453508316695 \\ H & -0.41010723140260 \\ H & -1.42255862242347 \\ H & -1.00421853741808 \\ H & 0.64544694565183 \\ \end{array} $	-6.17713647333709 -6.5831198013535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.15140434147396	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859
$ \begin{array}{c} \hbox{C} 0.49459548215242 \\ \hbox{H} 0.52430533690353 \\ \hbox{H} 1.14137584050426 \\ \hbox{H} 0.84758362703589 \\ \hbox{C} -0.39035122027211 \\ \hbox{H} 0.04453508316695 \\ \hbox{H} -0.41010723140260 \\ \hbox{H} -1.42255862242347 \\ \hbox{H} -1.00421853741808 \\ \hbox{H} 0.64544694565183 \\ \hbox{H} 0.59350406930491 \end{array} $	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -4.040587637082787 -2.8356592478291 -4.28500931591561 -4.95626140449838 -5.15140434147396 -2.4603878536367	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943
$\begin{array}{c} C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ H & 0.84758362703589 \\ C & 0.39035122027211 \\ H & -0.04453508316695 \\ H & -0.41010723140260 \\ H & -1.42255862242347 \\ H & -1.00421853741808 \\ H & 0.64544694565183 \\ H & 0.59350406930491 \\ C & -1.4636306444147 \end{array}$	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.911305436227 -2.83565924478291 -4.28500931591561 -4.95562160449838 -5.15140434147396 -2.460389785356367	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980
$ \begin{array}{c} C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ H & 0.84758362703589 \\ C & 0.39035122027211 \\ H & -0.04453508316695 \\ H & -0.41010723140260 \\ H & -1.42255862242347 \\ H & -1.00421853741808 \\ H & 0.64544694565183 \\ H & 0.59350406930491 \\ C & -1.46363606444147 \\ C & -2.1614052927744 \\ \end{array} $	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.9113054362787 -4.04058763708827 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.1514043147396 -2.46038978536367 -3.86634993801557 -3.86634993801557	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16664578486243
C 0.49459548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C 0.39035122027211 H 0.04453508316695 H 0.4410723140260 H 1.42255862242347 H 1.00421853741808 H 0.64544694565183 H 0.59350406930491 C -1.46363606444147 C -2.1144527321010	-6.17713647333709 -6.58311980133535 -6.75669594433612 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291 -4.25560140449838 -5.15140434147396 -2.46038978536367 -3.686634993801557 -3.21677321731649	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.655580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 2.406647358846245
$ \begin{array}{c} C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ H & 0.84758362703589 \\ C & 0.39035122027211 \\ H & -0.04453508316695 \\ H & -0.41010723140260 \\ H & -1.42255862242347 \\ H & -1.00421853741808 \\ H & 0.64544694565183 \\ H & 0.59350406930491 \\ C & -1.46363606444147 \\ C & -2.114453973391191 \\ U & 0.66752220714 \\ \end{array} $	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -2.83565924478291 -4.28500931591561 -4.28500931591561 -2.46038978536367 -3.68634993801557 -3.21677321731649 -1.85418651494572 -1.85418651494572	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 -2.49660073554519
$ \begin{array}{l} C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ H & 0.84758362703589 \\ C & -0.39035122027211 \\ H & 0.04453508316695 \\ H & -0.41010723140260 \\ H & -1.42255862242347 \\ H & 1.00421853741808 \\ H & 0.64544694565183 \\ H & 0.65350406930491 \\ C & -1.46363606444147 \\ C & -2.11635973391191 \\ H & -2.65687526392124 \\ \end{array} $	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.9113054362278 -4.04058763708827 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.15140434147396 -2.46038785356367 -3.68634993801557 -3.21677321731649 -1.85418651494572 -1.46027413651400	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.065556047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198
$ \begin{array}{c} \mbox{C} 0.49459548215242 \\ \mbox{H} 0.52430533690353 \\ \mbox{H} 1.14137584050426 \\ \mbox{H} 0.84758362703589 \\ \mbox{C} 0.39035122027211 \\ \mbox{H} -0.04453508316695 \\ \mbox{H} -0.41010723140260 \\ \mbox{H} -1.0421853741808 \\ \mbox{H} 0.64544694565183 \\ \mbox{H} 0.59350406930491 \\ \mbox{C} -1.1643506044147 \\ \mbox{C} -2.16140529227744 \\ \mbox{C} -2.11453973391191 \\ \mbox{H} -2.65687526392124 \\ \mbox{H} -2.74401530365918 \\ \end{array} $	$\begin{array}{r} -6.17713647333709\\ -6.58311980133535\\ -6.75669594453612\\ -6.34413312543620\\ -3.91130543622787\\ -2.83565924478291\\ -4.28500931591561\\ -4.95626140449838\\ -5.15140434147396\\ -2.46038978536367\\ -3.68634993801557\\ -3.21677321731649\\ -1.85418651494572\\ -1.46027413651401\\ -3.90978829278450\end{array}$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06555047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173
$ \begin{array}{l} \hline C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ H & 0.84758362703589 \\ C & 0.39035122027211 \\ H & -0.04453508316695 \\ H & -0.41010723140260 \\ H & -1.42255862242347 \\ H & -1.00421833741808 \\ H & 0.64544694565183 \\ H & 0.59350406930491 \\ C & -1.46363606444147 \\ C & -2.16414694565183 \\ H & 0.529227744 \\ C & -2.11453973391191 \\ H & -2.65687526392124 \\ H & -2.74401530365918 \\ H & -1.48127383040252 \\ \end{array} $	-6.17713647333709 -6.58311980133535 -6.75669594435312 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291 -4.28500931591561 -4.2850214748291 -4.2850214744828 -2.46038978536367 -3.68634993801557 -3.21677321731649 -1.85418651494572 -1.46027413651401 -3.90978829278450 -4.74298216899484	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558486245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495
$ \begin{array}{c} \hline c \ .49459548215242 \\ H \ .0.52430533690353 \\ H \ .14137584050426 \\ H \ .0.84758362703589 \\ C \ .0.39035122027211 \\ H \ .0.04455308316695 \\ H \ .0.41010723140260 \\ H \ .1.42255862242347 \\ H \ .1.04214853741808 \\ H \ .0.64544694565183 \\ H \ .0.59350406930491 \\ C \ .2.16140529227744 \\ C \ .2.16140529227744 \\ C \ .2.11453973810191 \\ H \ .2.65687526392124 \\ H \ .2.74401530365918 \\ H \ .1.48127383040252 \\ H \ .1.9825910047105 \\ \end{array} $	$\begin{array}{c} -6.17713647333709\\ -6.58311980133535\\ -6.75669594453612\\ -6.34413312543620\\ -3.9113024362278\\ -4.04058763708827\\ -2.83565924478291\\ -4.28500931591561\\ -4.95526140449838\\ -5.15140434147396\\ -2.46038978536367\\ -3.2663493801557\\ -3.21677321731649\\ -1.85418651494572\\ -1.46027413651401\\ -3.90978829278450\\ -4.74298216899484\\ 0.80916821245017\end{array}$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06555047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495 -2.66282925162534
$ \begin{array}{l} C & 0.49459548215242 \\ H & 0.52430533690353 \\ H & 1.14137584050426 \\ 0.84758362703589 \\ C & 0.39035122027211 \\ H & -0.04453508316695 \\ H & -4.1010723140260 \\ H & -1.42255862242347 \\ H & -1.00421853741808 \\ H & 0.64544694565183 \\ H & 0.59350406930491 \\ C & -1.46363606444147 \\ C & -2.114453973391191 \\ H & -2.65687526392124 \\ H & -2.744015303659118 \\ H & -1.48127383040252 \\ H & -1.98059610047105 \\ H & -0.23561095678447 \\ \end{array} $	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.15140434147396 -2.46038978536367 -3.68634993801557 -3.21677321731649 -1.85418651494572 -1.46027413651490 -3.90978829278450 -4.74298216899484 0.80916821245017 0 55828329141344	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.0655604779980 -2.16064558846245 -2.49660073554519 -3.35370499338198 -2.76713747189173 -0.81406592965495 -2.66282925162534 -2.62132021651254
C 0.49459548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C -0.39035122027211 H -0.04453508316695 H 0.44101723140260 H -1.42255862242347 H -1.00421853741808 H 0.65454694565183 H 0.59350406930491 C -1.46363606444147 C -2.16140529227744 C -2.116140529227744 H -2.65687526392124 H -2.65687526392124 H -2.74401530365918 H -1.48127383040252 H -1.98059610047105 H -0.22316095678457 C -2.30637684477	-6.17713647333709 -6.58311980133535 -6.75669594433612 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83563924478291 -4.95626140449838 -5.15140434147396 -2.46038978536367 -3.266149493801557 -3.2667321731649 -1.854186514901 -3.90978829278450 -4.74298216899484 0.80916821245017 0.55828329141344 144129758447778	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 -2.49660073554519 -3.3537049938198 -2.76713747189173 -0.81406592965495 -2.66282925162534 -2.66282925162534 -2.6123029163126 -0.11965645048255
C 0.49459548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C 0.39035122027211 H -0.04453508316695 H -0.41010723140260 H -1.42255862242347 H -1.00421853741808 H 0.64544694565183 H 0.59350406930491 C -1.46363606444147 C -2.114452973391191 H -2.65687526392124 H -2.74401530365918 H -1.48127383040252 H -1.98059610047105 H -0.22316095678457 C -2.3103736814772 C -2.31053736814772	$\begin{array}{l} -6.17713647333709\\ -6.5831198013353\\ -6.75669594353612\\ -6.34413312543620\\ -3.91130543622787\\ -4.04085763708827\\ -2.83565924478291\\ -4.28500931591561\\ -4.95626140449838\\ -5.15140434147396\\ -2.46038978536367\\ -3.68634993801557\\ -3.68634993801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.46843983801557\\ -3.4684398636634\\ -3.49843839801557\\ -3.4684398636634\\ -3.4984383986557\\ -3.4884383986557\\ -3.4884383986557\\ -3.4884383986557\\ -3.4884383986557\\ -3.4884383986557\\ -3.4884583986558\\ -3.4884586566666\\ -3.4884586566666\\ -3.4884586666666\\ -3.488456666666\\ -3.4884566666666\\ -3.4884566666666\\ -3.488456666666\\ -3.488456666666666\\ -3.488456666666666\\ -3.4884566666666666\\ -3.488456666666666666\\ -3.488456666666666666666666666666666666666$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 2.49660073554519 -3.35370499388198 -2.76713747189173 0.81406592965495 -2.66282925162534 -2.6213029163126 0.11965645048255
$ \begin{array}{l} \label{eq:constraints} C & 0.49459548215242 \\ \mbox{H} & 0.52430533690353 \\ \mbox{H} & 1.14137584050426 \\ \mbox{H} & 0.84758362703589 \\ \mbox{C} & 0.39035122027211 \\ \mbox{H} & 0.04453508316695 \\ \mbox{H} & -1.42255862242347 \\ \mbox{H} & -1.42255862242347 \\ \mbox{H} & -1.42255862242347 \\ \mbox{H} & -1.46363606444147 \\ \mbox{C} & -2.1614694565183 \\ \mbox{H} & 0.65454694565183 \\ \mbox{H} & 0.59350406930491 \\ \mbox{C} & -2.16140529227744 \\ \mbox{C} & -2.16140529227744 \\ \mbox{C} & -2.16140529227744 \\ \mbox{C} & -2.16140529227744 \\ \mbox{H} & -2.74401530365918 \\ \mbox{H} & -1.48127383040252 \\ \mbox{H} & -1.88127383040252 \\ \mbox{H} & -1.98059610047105 \\ \mbox{H} & -0.2316095678457 \\ \mbox{C} & -2.0367366814772 \\ \mbox{C} & -2.1145530889302 \\ \mbox{C} & -2.11345530898302 \\ \mbox{H} & -2.7400530367988370 \\ \mbox{C} & -2.11345530898302 \\ \mbox{C} & -2.1145538425384252 \\ \mbox{C} & -2.114553842534284254 \\ \mbox{C} & -2.114553842542424444444444444444444444444444$	-6.17713647333709 -6.58311980133535 -6.75669594435312 -6.34413312543620 -3.91130543622787 -4.04058763708827 -2.83565924478291 -4.28500931591561 -4.2850214748291 -4.28500931591561 -2.46038978536367 -3.66634993801557 -3.21677321731649 -1.85418651494572 -1.46027413651401 -3.90978829278450 -3.90978829278450 -3.92078829218499484 0.80916821245017 0.5582329141344 1.41129754647778 1.7138749758614778	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495 -2.66282925162534 -2.6628292516254 -2.1096545048255 1.35022200020878
$ \begin{array}{l} \label{eq:constraints} C & 0.49439548215242 \\ \mbox{H} & 0.52430533690353 \\ \mbox{H} & 1.14137584050426 \\ \mbox{H} & 0.84758362703589 \\ \mbox{C} & 0.39035122027211 \\ \mbox{H} & -0.04453508316695 \\ \mbox{H} & -0.41010723140260 \\ \mbox{H} & -1.0421853741808 \\ \mbox{H} & 0.64544694565183 \\ \mbox{H} & 0.645544694565183 \\ \mbox{H} & 0.645544694565183 \\ \mbox{H} & 0.65752639212744 \\ \mbox{C} & -2.1144523973391191 \\ \mbox{H} & -2.65687526392124 \\ \mbox{H} & -2.74401530365918 \\ \mbox{H} & -1.98059610047105 \\ \mbox{H} & -0.22316095678457 \\ \mbox{C} & -2.11345030898302 \\ \mbox{H} & -1.06591073848731 \\ \mbox{H} & -1.065910738$	$\begin{array}{r} -6.17713647333709\\ -6.58311980133533\\ -6.75669594453612\\ -6.34413312543620\\ -3.91130543622787\\ -2.83565924478291\\ -4.28500931591561\\ -4.9562160449838\\ -5.15140434147396\\ -2.46038978536367\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.68634993801557\\ -3.6863493801557\\ -3.6863493801557\\ -3.6863493801557\\ -3.6863493214341\\ -4.1928216821245017\\ 0.55828329141344\\ 1.44129754647778\\ 1.71387497586144\\ 1.06948650167499\end{array}$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 1.28114449770978 1.281534449770978 1.265580138321859 1.25344853432943 -1.06556047779880 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495 -2.62123029163126 -0.11965645048255 1.35022200020878
$ \begin{array}{l} \hline \begin{array}{l} \label{eq:constraints} \label{eq:constraints} \\ \mbox{C} 0.49459548215242 \\ \mbox{H} 0.52430533690353 \\ \mbox{H} 1.14137584050426 \\ \mbox{H} 0.84758362703589 \\ \mbox{C} 0.39035122027211 \\ \mbox{H} 0.04453508316695 \\ \mbox{H} 0.41010723140260 \\ \mbox{H} 0.454561833741808 \\ \mbox{H} 0.6454694565183 \\ \mbox{H} 0.59350406930491 \\ \mbox{C} 1.146363606444147 \\ \mbox{C} -2.1614694565183 \\ \mbox{H} 0.59350406930491 \\ \mbox{C} 2.16140522227744 \\ \mbox{C} -2.16140522227744 \\ \mbox{C} -2.1614052222744 \\ \mbox{C} -2.1614052222744 \\ \mbox{C} -2.1614052222744 \\ \mbox{C} -2.1614052227744 \\ \mbox{C} -2.161405222774 \\ \mbox{C} -2.1614059227747 \\ \mbox{C} -2.1614503068914772 \\ \mbox{C} -2.10367366814772 \\ \mbox{C} -2.1036871686347712 \\ \mbox{C} -0.88871586574128 \\ \mbox{C} -0.88871586574128 \\ \mbox{C} -0.88871586574128 \\ \mbox{C} -2.1614574762 \\ \mbox{C} -2.1614574762 \\ \mbox{C} -2.1614574762 \\ \mbox{C} -2.1614574762 \\ \mbox{C} -2.161457472 \\ \mbox{C} -2.1614574762 \\ \mbox{C} -2.161457476 \\ \mbox{C} -2.11345030898302 \\ \mbox{C} -2.1134503088731 \\ \mbox{C} -0.88871586574128 \\ \mbox{C} -2.161457476 \\ \mbox{C} -2.16145767476 \\ \mbox{C} -2.161457476 \\ \mbox{C} -2.161457476 \\ \mbox{C} -2.16145767476 \\ \mbox{C} -2.1614576747676 \\ \mbox{C} -2.16145767476 \\ \mbox{C} -2.1614576747676 \\ \mbox{C} -2.161457676767676 \\ \mbox{C} -2.16147767676767676767676767676$	-6.17713647333709 -6.58311980133535 -6.75669594453612 -6.34413312543620 -3.91130543622787 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.15140434147396 -2.46038978536367 -3.68634993801557 -3.68634993801557 -3.21677321731649 -1.85418651494572 -1.46027413651401 -3.9097882278450 -4.74298216899484 0.80916821245017 0.55828329141344 1.06348650167499 1.14837509794759	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.065560138321859 2.216064558846245 -2.49660073554519 -3.35370499388198 -2.67613747189173 -0.81406592965495 -2.66282925162534 -2.62123029163126 -0.11965645048255 1.35022200020878 1.9191925232188 3.27630441806711
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$ \begin{array}{l} \label{eq:constraints} \begin{array}{l} \mbox{C} 0.49439548215242 \\ \mbox{C} 0.49439548215242 \\ \mbox{H} 0.52430533690353 \\ \mbox{H} 1.14137584050426 \\ \mbox{H} 0.84758362703589 \\ \mbox{C} 0.39035122027211 \\ \mbox{H} -0.04453508316695 \\ \mbox{H} -0.41010723140260 \\ \mbox{H} -1.004218537411808 \\ \mbox{H} 0.64544694565183 \\ \mbox{H} 0.1456372639212744 \\ \mbox{C} -2.16140529227744 \\ \mbox{C} -2.16140529227744 \\ \mbox{C} -2.163752639212744 \\ \mbox{H} -2.74401530365918 \\ \mbox{H} -1.98059610047105 \\ \mbox{H} -2.2316095678457 \\ \mbox{C} -2.11345030898300 \\ \mbox{H} -1.2653912852925848 \\ \mbox{C} 0.47660694766652 \\ \mbox{C} 1.92579902437300 \\ \mbox{C} 1.92579902437310 \\ \mbox{C} 1.92579902437300 \\ \mbox{C} 1.925799040740 \\ \mbox{C} 1.925799040740 \\ \mbox{C} 1.925799040740 \\ \mbox{C} 1.925799040740 \\ \mbox{C} 1.925799047470 \\ \mbox{C} 1.925799047740 \\ \mbox{C} 1.925799047740 \\ \mbox{C} 1.925799047740 \\ \mbox{C} 1.925794740 \\$	$\begin{array}{l} -6.17713647333709\\ -6.58311980133533\\ -6.75669594453612\\ -6.34413312543620\\ -3.91130543622787\\ -2.83565924478291\\ -4.28500931591561\\ -4.9562160449838\\ -5.15140434147396\\ -2.4603878535637\\ -3.68634993801557\\ -3.21677321731649\\ -1.85418651494572\\ -1.46027413651401\\ -3.90978229278450\\ -4.74298216899484\\ 1.4812954637788\\ -1.4827413651401\\ -3.90978829278450\\ -4.74298216899484\\ 1.48129754647778\\ 1.71387497586144\\ 1.06948650167499\\ 1.14837509794759\\ 0.43371390478205\\ 0.27398539039372\\ 1.1119166300638511\\ -0.36283971987124\end{array}$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.66282925162534 -2.66282925162534 -2.66282925162534 -2.66282925162534 -3.6520020878 1.91919925232188 3.27630441806711 3.79002814092383 5.19078987431925 5.70682985196272 7.17203442522543 7.26048645818134
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$ \begin{array}{l} \hline \begin{array}{l} \hline \begin{array}{l} 0.49439548215242\\ \hline \begin{array}{l} 0.52430533690353\\ \hline \begin{array}{l} 1.14137584050426\\ \hline \begin{array}{l} 0.84758362703589\\ \hline \begin{array}{l} 0.39035122027211\\ \hline \begin{array}{l} 0.044355308316695\\ \hline \begin{array}{l} 0.44153508316695\\ \hline \begin{array}{l} 0.41010723140260\\ \hline \begin{array}{l} 1.42255862242347\\ \hline \begin{array}{l} 1.10421853741808\\ \hline \begin{array}{l} 0.64544694565183\\ \hline \begin{array}{l} 0.59350406930491\\ \hline \begin{array}{l} c& -1.4635306044147\\ \hline \begin{array}{l} c& -2.16140529227744\\ \hline \begin{array}{l} c& -2.16140529227744\\ \hline \begin{array}{l} -2.65630644147\\ \hline \begin{array}{l} c& -2.16140529227744\\ \hline \begin{array}{l} -2.65630644147\\ \hline \begin{array}{l} c& -2.1614053973391191\\ \hline \begin{array}{l} 1& -2.6565726392124\\ \hline \begin{array}{l} 1.98059610047105\\ \hline \begin{array}{l} 0.022316095678457\\ \hline \begin{array}{l} c& -2.30637366814772\\ \hline \begin{array}{l} c& -2.30637366814772\\ \hline \begin{array}{l} c& -2.30637366814772\\ \hline \begin{array}{l} c& -2.30637366814772\\ \hline \begin{array}{l} c& -2.113453030898302\\ \hline \begin{array}{l} 0.135558292258488\\ \hline \begin{array}{l} 0& 0.13555829225848731\\ \hline \begin{array}{l} c& -0.88871586574128\\ \hline \begin{array}{l} 0.1355829225848702\\ \hline \begin{array}{l} 1.26331802972900\\ \hline \begin{array}{l} 2.16233430251316\\ \hline \begin{array}{l} 2.76789082688702\\ \hline 1.043415164088211\\ \hline \begin{array}{l} c& 1.37910600212168\\ \hline \begin{array}{l} 2.2431651310227\\ \hline \end{array} \end{array} \end{array} \right $	$\begin{array}{l} -6.17713647333709\\ -6.58311980133535\\ -6.75669594433612\\ -6.34413312543620\\ -3.91130543622787\\ -4.04058763708827\\ -2.83565924478291\\ -4.95626140449838\\ -5.15140434147396\\ -2.46038978536367\\ -3.2663493801557\\ -3.2663493801557\\ -3.2663493801557\\ -3.2663493801557\\ -3.2663493801557\\ -3.2663493801557\\ -3.2663493801557\\ -3.2663493801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.264393801557\\ -3.26329714356144\\ -1.06948650167499\\ -0.43371390478205\\ 0.27398539039372\\ -1.1191663006353\\ 0.70714657038511\\ -0.36233971987124\\ -2.7122642964358\\ 0.91139314363859\\ 2.61704048800512\\ -2.93334882691324\\ \end{array}$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.065556047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.8140659965495 -2.66282925162534 -2.62282925162534 -2.62282925162554 1.3502200020878 1.91919925232188 3.27630441806711 3.79002814092383 5.19778987431925 5.70682985196272 7.17203442522543 7.26048645818134 7.59426595065460 7.79526931255793 5.62336004711335 5.97706206837366
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C 0.49439548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C 0.39035122027211 H -0.04453508316695 H -0.41010723140260 H -1.42255862242347 H -1.00421853741808 H 0.64544694565183 H 0.54544694565183 H 0.54544694565183 H 0.54544694565183 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -0.22316095678457 C -2.30637366814772 C -2.11345030898302 N -1.06591073847313 C -0.88871586574128 N 0.13555829225848 C 0.47660694766552 C 1.68318632972900 C 1.92579992437300 H 2.16253430251316 H 2.76789082688702 H 0.04341516408321 C -3.39478261310227 H 1.5801365225415 H 0.52349738213126 C 2.93487686447659 H 3.16455607967888 H 2.80466769525138 H 3.80917036797437 H 0.040425483740673 H 0.70925968701426 H 0.6344452752902440 C -2.8132646717425	-6.17713647333709 -6.58311980133535 -6.75669594435612 -6.34413312543620 -3.91130543622787 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.15140434147396 -2.46038978536367 -3.68634993801557 -3.68634993801557 -3.21677321731649 -1.85418651494572 -1.46027413651401 -3.90978829278450 -4.74298216899484 1.7438749786144 1.66948650167499 1.14837509794759 0.43371390478205 0.627394539039372 1.11191663006353 0.70714657038511 1.06948650167499 1.14837509794759 0.43371390478205 0.627394739188124 2.88715899836762 0.79501941744588 -0.28051039794449 2.88715899836762 0.79501941744588 -0.28051039794439 1.1524180366317 1.32704835569528 0.48351523697803 -0.79068596718182 -0.15351621171742	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495 -2.66282925162534 -2.66282925162534 -2.66282925162534 -2.6213029163126 -0.11965645048255 1.3502200020878 1.91919925232188 3.27630441806711 3.7900281409283 5.19778987431925 5.70682985196272 7.17203442522543 7.2604845818134 7.59426595065460 7.79526931255793 5.62936000471335 5.97706206837366 4.60072751638282 6.2644260968105 4.87042580954227 4.88084654154331 3.82655781864908 5.26866798498602 5.81829866083422 5.3514325433643 3.09649975812367
C 0.49439548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C 0.39035122027211 H 0.04453508316692 H 0.41010723140260 H 1.42255862242347 H 1.00421853741808 H 0.64544694565183 H 0.59350406930491 C -2.16140529227744 C -2.16140529227744 C -2.16140529227744 C -2.16140529227744 H -2.65467526392124 H -2.65467526392124 H -2.65467526392124 H -2.25405610047105 H 0.22316095678457 C -2.31043736814772 C -2.1145303898302 N -1.06591073848731 C -0.88871586574128 N 0.1355529225848 C 0.47660694766652 C 1.63318632972900 C 1.9257992437300 H 2.16253430251316 H 2.76789082688702 H 1.04341516408321 C 1.37910600212168 H 2.24231651310227 H 1.1580135225415 H 0.52349738213126 C 2.93487686447659 J 3.16455607967888 H 2.80466769525138 H 3.80917036797497 H 0.40422483740673 H 0.70925968701426 H 0.63446327529906 C -1.77351299962440 C -2.81396467171163	-6.17713647333709 -6.5831198013353 -6.75669594453612 -6.34413312543620 -3.911305436278 -4.40058763708827 -2.83565924478291 -4.28500931591561 -4.95626140449838 -5.15140434147396 -2.460389785356367 -3.21677321731649 -1.85418651494572 -1.46027413651401 -3.90978229278450 -4.74298216899348 0.80916821245017 0.55828329141344 1.4129754647778 0.43371390478205 0.2739853903972 1.11191663006353 0.2739853903972 1.11191663006353 0.2739853903972 1.11191663006353 0.273945801324 2.93334882691324 2.88715899836762 0.790485509524 2.93334882691324 2.88715899836762 0.7906596718182 -0.28051039744433	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495 -2.66282925162534 -3.6520020878 1.919925232188 3.27630441806711 3.7002214022383 5.19778987431925 5.70662985196272 7.17203442522543 7.26048645818134 7.59426595065460 7.79526931255793 5.6936000471335 5.97706206837366 4.60072751638282 6.26442669968105 4.87042580954227 4.88084654154331 3.82655781864908 5.26865798498603422 5.8182986083422 5.81829
C 0.49439548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C 0.39035122027211 H -0.04453508316695 H -0.41010723140260 H -1.42255862242347 H -1.00421853741808 H 0.64544694565183 H 0.54544694565183 H 0.54544694565183 H 0.54544694565183 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.74401530365918 H -2.316095678457 C -2.316095678457 C -2.3063736814772 C -2.1134503089802 N -1.065910738487313 C 0.476660694766552 C 1.68318632972900 C 1.92579992437300 H 2.0423430251316 H 2.76789082688702 H 1.04341516408231 C 1.37910600212168 H 2.24231651310227 H 1.580136525415 H 0.5234778251326 C 2.93487686447659 H 3.16455607967888 H 2.8046769525138 H 3.80917036797497 H 0.40425483740673 H 0.70925968701426 C -2.81386467171163 C -2.81386467171163 C -2.8138646717163	-6.17713647333709 -6.58311980133533 -6.75669594435612 -6.34413312543620 -3.91130543622787 -2.83565924478291 -4.28500931591561 -4.9562160449838 -5.15140434147396 -2.46038978535637 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.68634993801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -3.6863493801557 -0.7384539039372 -1.1191663006353 0.707947497954 2.93334882691324 -0.28871589836762 0.79501941744586 -0.28051039794449 -2.88715899836762 0.790615947497954 2.93334882691324 -0.28051039794449 -0.2805103794449 -0.2805103794449	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.25344853432943 -1.06556047779980 -2.16064558846245 2.49660073554519 -3.35370499388198 -2.76713747189173 0.81406592965495 -2.66282925162534 -2.62123029163126 -0.11965645048255 1.3502200020878 1.91919925232188 3.27630441806711 3.79002814092383 5.19778987431925 5.70682985196272 7.17203442522543 7.26048645818134 7.59426595065460 7.79526931255793 5.62336000471335 5.97706206837366 4.60072751638282 6.264424500968105 4.87042580954227 4.88084654154331 3.82655781864908 5.26865798498602 5.818429866083422 5.3514325433068 3.09649975812367 4.05961632817874 3.44969754330068
C 0.49439548215242 H 0.52430533690353 H 1.14137584050426 H 0.84758362703589 C 0.39035122027211 H -0.04453508316695 H -0.41010723140260 H -1.42255862242347 H -1.00421853741808 H 0.64544694565183 H 0.59350406930491 C -1.4636306044147 C -2.16140529227744 C -2.11453973391191 H -2.65687526392124 H -2.74401530365918 H -1.48127383040252 H -0.22316095678457 C -2.3063736614772 C -2.1145303898302 N -1.06591073848731 C -0.88871586574128 N 0.13555829225848 C 0.47660694766652 C 1.68318632972900 C 1.92579992437300 H 2.16253430251316 H 2.76789082688702 H 1.04341516408321 C 1.37910600212168 H 2.24314551310227 H 1.15801365225415 H 0.52349738213126 C 2.93487686447659 H 3.16455607967888 H 2.80466769525138 H 3.80917036794977 H 0.40425483740679 H 0.634453729906 C -1.77351299962440 C -3.30449319334447 H -3.82441800707923	$\begin{array}{l} -6.17713647333709\\ -6.5831198013533\\ -6.756695944353612\\ -6.344133125436200\\ -3.9113024362277\\ -2.83565924478291\\ -4.28500931591561\\ -4.95626140449838\\ -5.15140434147396\\ -2.46038978536367\\ -3.26634993801557\\ -3.26634993801557\\ -3.26634993801557\\ -3.26634993801557\\ -3.26634993801557\\ -3.264773217316494572\\ -1.46027413651401\\ -3.90978829278450\\ -4.74298216899484\\ 0.80916821245017\\ 0.55828329141344\\ 1.44129754647778\\ 1.71387497586144\\ 1.06948650167499\\ 1.14837509794759\\ 0.43371390478205\\ 0.27398539039372\\ 1.1191663006353\\ 0.27398539039372\\ 1.1191663006353\\ 0.27398539039372\\ 1.1191663006353\\ 0.27398539039372\\ 2.907594749754\\ 2.93334882691324\\ 2.8715899836762\\ -2.28051039794443\\ 1.1524180366317\\ 1.32704835569528\\ 0.48381523697803\\ -0.79068596718182\\ -0.1535162117172\\ 1.941615985413\\ 2.600859718182\\ -0.1535162117172\\ 1.941615985413\\ 2.60085712205692\\ 2.5002357603543\\ 3.00788434681679\\ \end{array}$	3.11112084393937 3.03866863727053 2.43735052278988 4.13727888947026 3.74087498305337 4.77552617061101 3.52183094005276 3.68529640343430 1.28114449770978 0.65580138321859 1.251344853432943 -1.06556047779980 -2.16064558846245 -2.49660073554519 -3.35370499388198 -2.76713747189173 -0.81406592965495 -2.66282925162534 2.62282925162534 2.62123029163126 -0.11965645048255 1.3502220002878 3.27630441806711 3.79002814092383 5.19778987431925 5.70682985196272 7.17203442522543 7.26048645818134 7.59426595065460 7.79526931255793 5.6236000471335 5.97706206837366 4.60072751638282 6.26442660968105 4.87042580954227 4.88084654154331 3.8265781864908 5.81829866083422 5.35143235433643 3.09649975812367

H -1.61997/57223807	2.02545/04868169	5.13128444988550
H -2.89782242340439	2.23737618903646	-0.60003451409000
H -2.86472921308004	0.50011691004301	-0.23208359145450
C -0.30323041573250	2.54261419994718	-1.04214332391344
C 1 15212080499283	2 29182425195200	-1 35835916154869
N 1 67476151371148	1 18273826106302	0 78190251475112
C 206751629721149	0.92507440277947	1 04960651990017
C 2.96/31038/31148	0.82397449277847	-1.04800031889917
N 3.38815770213843	-0.35282202369320	-0.52914106115021
H 2.69177940051581	-0.84431766648869	0.04319020387215
C 3.78222858701510	1.67828323358135	-1.84216600116015
C 3 23866735813770	2 82399333481736	-2 38738707389773
C 1 9969040000952	2 12040162668025	2.17170761706770
C 1.88080409909855	3.13940103008923	-2.1/1/9/01/90//9
H 1.42659352382042	4.01389/15201652	-2.626/603084/163
H 3.85896481612149	3.47262085800309	-3.00526143627272
H 4.81621114379079	1.41320055471866	-2.04193317667399
H -0 78578593771997	3 12005448278914	-1 84786840402787
H _0 30078405870857	3 12040053312256	-0 11536175337315
C 4 7378507495679657	0.02574507200808	0.00011100000770
C 4.72785074895323	-0.925/450/209808	-0.60811166949779
C 4.907/3262703912	-2.08669968582599	-1.62512651471592
C 4.63879549345082	-1.60369170721147	-3.05970417616678
H 3.61742567866546	-1.21452445746035	-3.16999555704160
H 5 34333610812845	-0.81448003112511	-3 35827497552197
H 4 75528019408865	-2 43296050760660	-3 77046262960232
11 4.75528019408805	-2.43290030700000	-3.77040202900232
C 3.951932166/3899	-3.24112092443878	-1.2//3928935/2//
H 2.90019427480584	-2.93796552213287	-1.37281094378063
H 4.11364465895389	-4.08898425500017	-1.95642184078687
H 4.11547306100402	-3.59993651799501	-0.25084203070709
C 6 36461315897833	-2 56828410200203	-1 50314580869775
Н 6 55/0620020007	-3 30655021421087	-2 1082241546006
H 0.33490308082837	-3.39033021421087	-2.19823413408008
H /.0/564966033604	-1./6425405028116	-1./4156008588935
H 6.58644378392344	-2.92735892490452	-0.48797000593981
H 5.45010820395206	-0.12890399816519	-0.82812986356304
H 4 98152900943802	-1 30315635016133	0 39459368603009
11 1.901029009 19002	1.50515055010155	0.07 107000000000
Table \$16 Contagion as	andinatas (Å) for CEE	Defeeds UVADON
Table S16. Cartesian co	ordinates (A) for CSL	Relicoue UKARON
Atom X	Y	L
Cu 0.03265785837909	0.00648310657152	-0.05390672376131
S 1.20244776319695	-1.23308902489908	-1.84934797311315
C 2 31678843541113	-2 38430023674110	-0 91358203292444
C 3 25516445205167	-3 17858903293085	-1 81127933299171
11 2 84866052600507	2 86024062005510	1 10622724206850
H 3.84800033000307	-5.80924005005519	-1.19032734290830
H 2.70091987742090	-3.7/052350/06414	-2.54907942120658
H 3.96202910617939	-2.53418770146838	-2.34937519687396
H 1.61226393243281	-3.03809992175648	-0.38503490965026
H 2 85090111719090	-1 80394651763289	-0 15182385685972
C 2 24060155242740	0 15261972557392	2 27005780422002
C 2.34009133343749	1.00142022220407	1 102000204(0410
C 2.008209/20/8559	1.0814303332048/	-1.10300029469419
NT 1 0 (818050051081	1 5 (000 5000 10100	0 110 (00100 50 50 50
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$\begin{array}{l} {\rm N}\ 1.36717353251374}\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064555107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ -0.82310378284313\\ {\rm C}\ -2.16702388087503\\ {\rm H}\ -3.00242303703074\\ {\rm H}\ -2.25741645766201\\ {\rm H}\ -2.28290516906114\\ {\rm C}\ -0.73632408069528\\ {\rm H}\ -1.5745247106927\\ {\rm H}\ -0.78039739474396\\ {\rm H}\ 0.078039739474396\\ {\rm H}\ 0.076397393644740\\ {\rm H}\ -0.76397393644740\\ {\rm H}\ -0.76397393644740\\ {\rm H}\ -0.76397393644740\\ {\rm H}\ -0.51456948940017\\ {\rm H}\ -1.51456948940017\\ {\rm H}\ -1.51456948940017\\ {\rm H}\ -1.5245684874007\\ {\rm H}\ -1.52456848\\ {\rm H}\ -1.5745247168488\\ {\rm H}\ -1.5145684874007\\ {\rm H}\ -1.524568488\\ {\rm H}\ -1.514568484607\\ {\rm H}\ -1.514568488607\\ {\rm H}\ -1.514568488660\\ {\rm H}\ -1.514568488607\\ {\rm H}\ -1.514568886607\\ {\rm H}\ -1.51456886667\\ {\rm H}\ -1.5145688667\\ {\rm H}\ -1.51456868667\\ {\rm H}\ -1.51456868667\\ {\rm H}\ -1.51456868667\\ $	$\begin{array}{l} 1.56802580240128\\ 2.12882896081191\\ 1.03299847920164\\ -0.05568032826182\\ -1.0692987303373\\ -2.11499145868648\\ -3.33150618030967\\ -3.42480687503060\\ -3.42480687503060\\ -3.442815779354386\\ -4.1480260103398\\ -2.38393129481778\\ -2.2753818803979\\ -2.36579430886828\\ -1.30635355770883\\ -3.364781880528521646\\ -4.78988361670816\\ -4.78988361670816\\ -4.78988361670816\\ -4.78988361670816\\ -4.78988361670816\\ -4.78988361670816\\ -4.78988361670816\\ -4.828283254046\\ -3.46682438762012\\ \end{array}$	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933
$\begin{array}{l} {\rm N}\ 1.36717353251374}\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064505107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ -0.82310378284313\\ {\rm C}\ -2.16702388087503\\ {\rm H}\ -3.00242303703074\\ {\rm H}\ -2.28290516906114\\ {\rm C}\ -0.73632408069528\\ {\rm H}\ -1.57452547106927\\ {\rm H}\ 0.78037393474396\\ {\rm H}\ 0.19188916848929\\ {\rm C}\ -0.70299965669533\\ {\rm H}\ -0.780373934644704\\ {\rm H}\ 0.24846957514484\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ 1.30271282742586\\ {\rm H}\ 0.26050022476613\\ \end{array}$	$\begin{array}{l} 1.56802580240128\\ 2.12882896081191\\ 1.03299847920164\\ -0.05568032826182\\ -1.0692987303373\\ -2.11499145868648\\ -3.33150618030967\\ -3.42480687503060\\ -3.34478182931530\\ -3.4478182931530\\ -3.4478182931530\\ -3.447818293129481778\\ -2.29753818803979\\ -2.36579430886828\\ -2.38393129481778\\ -2.36019583232616\\ -4.78988361670816\\ -4.78988361670816\\ -4.78988361670816\\ -3.4682438757083907\\ -4.88091480593891\\ -4.92144328254046\\ -3.468243875(2012)\\ -4.17854997694668\end{array}$	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.85627670972933
$\begin{array}{l} {\rm N}\ 1.36717353251374\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064505107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ 0.82310378284313\\ {\rm C}\ 2.16702388087503\\ {\rm H}\ -3.00242303703074\\ {\rm H}\ -2.25741645766201\\ {\rm H}\ -2.25791516986\\ {\rm H}\ 0.15818916848292\\ {\rm C}\ -0.70299965669533\\ {\rm H}\ -0.76397393644740\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ -1.515697514848\\ {\rm H}\ 0.26050022476613\\ {\rm H}\ -0.25750757866661\\ {\rm H}\ -0.25750757866661\\ \end{array}$	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.58984450210265 5.57793371456792 3.85627670972933 2.62981390096151 1.72878854452120
$\begin{array}{l} {\rm N}\ 1.36717353251374\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064505107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ 0.082310378284313\\ {\rm C}\ 2.216702388087503\\ {\rm H}\ -3.00242303703074\\ {\rm H}\ -2.2820516906114\\ {\rm C}\ -0.73632408069528\\ {\rm H}\ -1.57452547106927\\ {\rm H}\ 0.7803739474339\\ {\rm H}\ 0.19188916848929\\ {\rm C}\ 0.70299965669533\\ {\rm H}\ 0.78037393744749\\ {\rm H}\ 0.218297393644740\\ {\rm H}\ 0.24846957514484\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ 1.30271282742568\\ {\rm H}\ 0.26050022476613\\ {\rm H}\ 0.257507578666661\\ {\rm C}\ 2.1924520837008\\ \end{array}$	$\begin{array}{l} 1.56802580240128\\ 2.1288280681191\\ 1.03299847920164\\ -0.05568032826182\\ -1.0692987303373\\ -2.11499145868648\\ -3.33150618030967\\ -3.42480687503060\\ -3.34478182931530\\ -3.44875779354386\\ -4.1480260103398\\ -2.38393129481778\\ -2.29753818803979\\ -2.36579430886828\\ -1.30635355770883\\ -2.36019583232616\\ -4.78988361670816\\ -4.78988361670816\\ -3.561878076699907\\ -4.88091480593891\\ -4.92144328254046\\ -3.46682438762012\\ -4.17854997694668\\ -2.02519758323955 \\ -0.97434100137578\end{array}$	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458
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$\begin{array}{l} {\rm N} \ 1.36717353251374 \\ {\rm C} \ 1.67547180021872 \\ {\rm C} \ 1.94586007917532 \\ {\rm N} \ 1.15022738342134 \\ {\rm C} \ 1.24064505107964 \\ {\rm N} \ 0.40415367237564 \\ {\rm C} \ 0.34950836519569 \\ {\rm C} \ -0.82310378284313 \\ {\rm C} \ 2.216702388087503 \\ {\rm H} \ 3.00242303703074 \\ {\rm H} \ -2.28290516906114 \\ {\rm C} \ 0.73632408069528 \\ {\rm H} \ -1.57452547106927 \\ {\rm H} \ -0.78039739474396 \\ {\rm H} \ 0.078039739474396 \\ {\rm H} \ 0.078039739474396 \\ {\rm H} \ 0.0729965669533 \\ {\rm H} \ -0.763973936447740 \\ {\rm H} \ 0.327128274256613 \\ {\rm H} \ -0.26050022476613 \\ {\rm H} \ 0.26050022476613 \\ {\rm H} \ -0.25750757866661 \\ {\rm C} \ 2.19245220837008 \\ {\rm C} \ 3.0092069963170 \\ {\rm C} \ 2.8663214494 \\ \end{array}$	1.56802580240128 2.1288280681191 1.03299847920164 -0.05568032826182 -1.06929873033373 -2.11499145868648 -3.33150618030967 -3.42480687503060 -3.4478182931530 -3.44875779354386 -4.14802601033398 -2.38393129481778 -2.36579430886828 -2.38393129481778 -2.36579430886828 -3.3619583232616 -4.78988361670816 -5.61878076699907 -4.88091480593891 -3.61682438762012 -4.17854997694668 -2.02519758523955 -0.97434109137578 0.13307730734306	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.7287885842180 3.75599469220458 3.84341442578426 2.093014744738
$\begin{array}{l} {\rm N}\ 1.36717353251374\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064505107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ 0.82310378284313\\ {\rm C}\ 2.216702388087503\\ {\rm H}\ -3.0024230370374\\ {\rm H}\ -2.225741645766201\\ {\rm H}\ -2.2820516906114\\ {\rm C}\ -0.73632408069528\\ {\rm H}\ -1.57452547106927\\ {\rm H}\ 0.07839739474396\\ {\rm H}\ 0.19188916848929\\ {\rm C}\ 0.70299965669533\\ {\rm H}\ 0.76397393644740\\ {\rm H}\ 0.2484695751444\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ 1.30271282742568\\ {\rm H}\ 0.25750757866661\\ {\rm C}\ 2.19245220837908\\ {\rm C}\ 3.00920699963170\\ {\rm C}\ 2.89638241489390\\ {\rm H}\ 1.514569429441925264\\ {\rm C}\ 3.00920699963170\\ {\rm C}\ 2.89638241489390\\ {\rm H}\ 3.566661\\ {\rm C}\ 3.00920699963170\\ {\rm C}\ 3.0092069963170\\ {\rm C}\ 3.0092000000\\ {\rm C}\ 3.0092000000000\\ {\rm C}\ 3.0000000000000000$	1.56802580240128 2.12882896081191 1.03299847920164 4.0.05568032826182 -1.0692987303373 -2.11499145868648 -3.33150618030967 -3.42480687503060 -3.34478182931530 -3.34478182931530 -3.34478182931530 -3.34478182931530 -3.34478182931530 -3.34478182931530 -3.34478182931530 -3.34679343086828 -2.36019583232616 -4.78988361670816 -5.61878076699907 -4.88091480593891 -4.92144328254046 -3.46682438762012 -4.17854997694668 -2.02519758523955 0.97434109137578	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458 3.84341442578426 2.90391474494738
$\begin{array}{l} {\rm N}\ 1.36717353251374}\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064555107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ -0.82310378284313\\ {\rm C}\ -2.16702388087503\\ {\rm H}\ -3.00242303703074\\ {\rm H}\ -2.25741645766201\\ {\rm H}\ -2.28290516906114\\ {\rm C}\ -0.73632408069528\\ {\rm H}\ -1.57452547106927\\ {\rm H}\ -0.78039739474396\\ {\rm H}\ 0.078039739474396\\ {\rm H}\ 0.078039739474396\\ {\rm H}\ 0.15188916848929\\ {\rm C}\ -0.76397393644740\\ {\rm H}\ 0.24846957514484\\ {\rm H}\ -1.51456948940017\\ {\rm H}\ 1.30271282742568\\ {\rm H}\ 0.26050022476613\\ {\rm H}\ -0.25757866661\\ {\rm C}\ 2.19245220837908\\ {\rm C}\ 3.00920699963170\\ {\rm C}\ 2.89638241489209\\ {\rm H}\ 3.52085443262974\\ \end{array}$	$\begin{array}{l} 1.56802580240128\\ 2.1288280681191\\ 1.03299847920164\\ -0.05568032826182\\ -1.0692987303373\\ -2.11499145868648\\ -3.33150618030967\\ -3.42480687503060\\ -3.42480687503060\\ -3.4478182931530\\ -3.44875779354386\\ -4.14802610133398\\ -2.38393129481778\\ -2.29753818803979\\ -2.36579430886828\\ -1.30635355770883\\ -2.36579430886828\\ -1.30635355770883\\ -2.3657943088628\\ -3.46882438762012\\ -4.78988516170816\\ -3.46682438762012\\ -4.17854997694668\\ -3.46682438762012\\ -4.17379680007279\\ 2.06280173734306\\ -1.13737680007279\\ 2.06280129511493\end{array}$	0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.54625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458 3.84341442578426 2.90391474494738
$\label{eq:constraints} \begin{array}{l} {\rm N}\ 1.36717353251374} \\ {\rm C}\ 1.67547180021872} \\ {\rm C}\ 1.94586007917532 \\ {\rm N}\ 1.15022738342134 \\ {\rm C}\ 1.24064505107964 \\ {\rm N}\ 0.40415367237564 \\ {\rm C}\ 0.34950836519569 \\ {\rm C}\ -0.82310378284313 \\ {\rm C}\ -2.16702388087503 \\ {\rm H}\ -3.00242303703074 \\ {\rm H}\ -2.28290516906114 \\ {\rm C}\ -0.73632408069528 \\ {\rm H}\ -1.57452547106927 \\ {\rm H}\ -0.78037939747396 \\ {\rm H}\ 0.19188916848929 \\ {\rm C}\ -0.70299965669533 \\ {\rm H}\ -0.78037937447396 \\ {\rm H}\ 0.24846957514484 \\ {\rm H}\ -1.51456948946017 \\ {\rm H}\ 1.30271282742568 \\ {\rm H}\ 0.26050022476613 \\ {\rm H}\ 0.25750757866661 \\ {\rm C}\ 2.19245220837908 \\ {\rm C}\ 3.00920699963170 \\ {\rm C}\ 2.89638241439297 \\ {\rm H}\ 3.52085443262974 \\ {\rm H}\ 3.73835209380879 \end{array}$	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458 3.84341442578426 2.903914774494738 2.96097500222532
$\begin{array}{l} {\rm N}\ 1.36717353251374 \\ {\rm C}\ 1.67547180021872 \\ {\rm C}\ 1.94586007917532 \\ {\rm N}\ 1.15022738342134 \\ {\rm C}\ 1.24064505107964 \\ {\rm N}\ 0.40415367237564 \\ {\rm C}\ 0.34950836519569 \\ {\rm C}\ 0.82310378284313 \\ {\rm C}\ 2.16702388087503 \\ {\rm H}\ -3.00242303703074 \\ {\rm H}\ -2.25741645766201 \\ {\rm H}\ -2.25741645766201 \\ {\rm H}\ -2.25245106927 \\ {\rm H}\ 0.73632408069528 \\ {\rm H}\ -1.57452547106927 \\ {\rm H}\ 0.76397393644740 \\ {\rm H}\ 0.19188916848929 \\ {\rm C}\ -0.70399965569533 \\ {\rm H}\ -0.763973937447496 \\ {\rm H}\ 0.19188916848929 \\ {\rm C}\ 0.76397514434 \\ {\rm H}\ -1.51456948946017 \\ {\rm H}\ 1.30271282742568 \\ {\rm H}\ 0.26550022476613 \\ {\rm H}\ 0.25750757866661 \\ {\rm C}\ 2.19245220837908 \\ {\rm C}\ 3.00920699963170 \\ {\rm C}\ 3.2092609963170 \\ {\rm H}\ 3.73835209380879 \\ {\rm H}\ 2.2632088108376 \\ \end{array}$	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 4.34503271854406 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458 3.84341442578426 2.90391474494738 2.90697500222532 4.65025965581055
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$\begin{array}{l} {\rm N}\ 1.36717353251374}\\ {\rm C}\ 1.67547180021872\\ {\rm C}\ 1.94586007917532\\ {\rm N}\ 1.15022738342134\\ {\rm C}\ 1.24064555107964\\ {\rm N}\ 0.40415367237564\\ {\rm C}\ 0.34950836519569\\ {\rm C}\ -0.82310378284313\\ {\rm C}\ -2.16702388087503\\ {\rm H}\ -3.00242303703074\\ {\rm H}\ -2.25741645766201\\ {\rm H}\ -2.28290516906114\\ {\rm C}\ -0.73632408069528\\ {\rm H}\ -1.57452547106927\\ {\rm H}\ -0.78039739474396\\ {\rm H}\ 0.078039739474396\\ {\rm H}\ 0.076397393644740\\ {\rm H}\ 0.24846957514484\\ {\rm H}\ -1.51456948946017\\ {\rm H}\ 1.30271282742568\\ {\rm H}\ 0.26050022476613\\ {\rm H}\ 0.257057866661\\ {\rm C}\ 2.19245220837908\\ {\rm C}\ 3.00920699963170\\ {\rm C}\ 2.89638214483209\\ {\rm H}\ 3.52085443262974\\ {\rm H}\ 3.73835209380879\\ {\rm H}\ 2.26320881803762\\ {\rm H}\ 2.252157787069680\\ {\rm H}\ 0.79028697062368\\ {\rm C}\ 0.62240176946237\\ {\rm C}\ 0.7959216909177\\ {\rm C}\ -0.7959216909177\\ \end{array}$	$\begin{tabular}{lllllllllllllllllllllllllllllllllll$	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.4625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458 3.84341442578426 3.90391474494738 2.90391474494738 2.90391474494738 2.90597500222532 4.65025965581055 4.49656242517612 0.84533490934559 1.22349310577957 -1.2730408265404 -0.78164512820158
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$\begin{array}{l} {\rm N} 1.36717353251374 \\ {\rm C} 1.67547180021872 \\ {\rm C} 1.94586007917532 \\ {\rm N} 1.15022738342134 \\ {\rm C} 1.24064505107964 \\ {\rm N} 0.40415367237564 \\ {\rm C} 0.34950836519569 \\ {\rm C} 0.482310378284313 \\ {\rm C} 2.16702388087503 \\ {\rm H} -3.00242303703074 \\ {\rm H} -2.2820516906114 \\ {\rm C} -0.73632408069528 \\ {\rm H} -1.57452547106927 \\ {\rm H} 0.78037939474396 \\ {\rm H} 0.19188916848929 \\ {\rm C} 0.70299965669533 \\ {\rm H} 0.78037939474396 \\ {\rm H} 0.282407393464470 \\ {\rm H} 0.24846957514484 \\ {\rm H} -1.51456948946017 \\ {\rm H} 1.30271282742586 \\ {\rm H} 0.26050022476613 \\ {\rm H} 0.25750757866661 \\ {\rm C} 2.19245220837098 \\ {\rm C} 3.0092069963170 \\ {\rm C} 2.89638241489390 \\ {\rm H} 3.52085443262974 \\ {\rm H} 3.7383209388076 \\ {\rm H} 0.7956921699077 \\ {\rm N} -3.20347431735088 \\ {\rm C} 0.62240176946257 \\ {\rm C} -0.79569216909177 \\ {\rm N} -1.37246677911365 \\ {\rm C} -2.68566148310029 \\ {\rm N} -3.203474131735088 \\ {\rm C} -5.56946118480584 \\ {\rm C} -5.0454322051225 \\ {\rm H} +4.13575461193042 \\ {\rm H} +4.81524625847981 \\ {\rm H} -5.79783988647827 \\ {\rm C} -6.8806535144479 \\ \end{array}$	1.56802580240128 2.12882896081191 1.03299847920164 4.005568032826182 -1.0692987303373 -2.11499145868648 -3.33150618030967 -3.42480687503060 -3.34478182931530 -3.44875779354386 -4.1480260103398 -2.38393129481778 -2.38393129481778 -2.38579430886828 -1.3063555770883 -2.36019583232616 -4.78988361670816 -4.78988361670816 -4.78988361670816 -4.78988361670816 -3.46824348762012 -4.17854997694668 -2.02519758523955 -0.97434109137578 0.02267340883056 -1.76339689805230 2.83202732005345 2.5607881282894978 2.5509811433 0.20257340883056 -1.76539689805230 2.83202732005345 2.5607881282894978 2.5509811433 0.20257340883056 -1.76339689805230 2.83202732005345 2.5607881282894978 2.55090113839633 2.70587104502622 1.5630881531443 1.58218226933678 0.4180383634191 0.202287360717 -0.46125978070938 -1.7230423755914 -2.48422520343182 -1.7230423755914	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.7559469220458 3.84341442578426 2.90391474494738 2.96097500222532 4.465025965581055 4.49656242517612 0.84533490934559 1.22349310577957 1.27304082605404 -0.78164512820158 -0.33495310034920 0.0677257739372 0.50409872024737 1.06476276505393 0.11901571602505 -0.3511355139703 -0.95827616676363 0.50158126142185 -0.9695737848124
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N 1.36717353251374 C 1.67547180021872 C 1.94586007917532 N 1.15022738342134 C 1.24064505107964 N 0.40415367237564 C 0.34950836519569 C -0.82310378284313 C -2.16702388087503 H -3.00242303703074 H -2.2820516906114 C -0.73632408069528 H -1.57452547106927 H -0.7803739474396 H 0.19188916848929 C -0.70299965669533 H -0.76397394764396 H 0.24846957514484 H -1.51456948946017 H .30271282742568 H 0.26050022476613 H -0.25750757866661 C 2.19245220837098 C 3.00920699963170 C 2.89638241483930 H 3.520854343262974 H 3.73835209380879 H 2.26320881083762 H 2.52157787069680 U 0.79028697062368 C 0.62240176946257 C -0.79569216909177 N -1.37246677911365 C 2.68566148310029 N -320347431735088 C 4.53244460237828 C -5.0454322051225 H -4.13575461193042 H -4.8152462584781 H -5.79783988647827 C -6.8606335414193	1.56802580240128 2.1288280681191 1.03299847920164 -0.05568032826182 -1.0692987303373 -2.11499145868648 -3.33150618030967 -3.42480687503600 -3.34478182931530 -3.44875779354386 -4.1480260103398 -2.38393129481778 -2.26579430886828 -1.3663555770883 -2.36019583223616 -4.78988361670816 -4.78988361670816 -5.61878076699907 -4.88091480593891 -4.92144328254046 -3.46682438762012 -4.17854997694668 -2.0251975823955 0.97434109137578 0.13307730734306 1.17379680007279 0.9243478251493 0.02267340883056 -1.76539689805230 0.20267340883056 -1.76539689805230 0.20267340883056 -1.76539689805230 0.20267340883056 -1.76539689805230 0.20267340883056 -1.76539689805230 0.202734075452 2.55090113839633 2.70887104502622 1.56308081531443 1.58218226953678 0.41808383634191 0.20728079607717 -0.46125978070938 -1.72300423755914 -2.8442520343182 -2.3367569428320 -1.72300423755914	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.77393371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.75599469220458 3.845341442578426 2.96097500222532 4.65025965581055 4.49656242517612 0.84533490934559 1.22349310577957 1.27304082605404 -0.7816412820158 -0.33495310034920 0.06772577393972 0.50409872024737 1.06476276505393 0.11901571602505 -0.35113551395703 -0.95827616676363 0.50158126142185 -0.93947243749
N 1.36717353251374 C 1.67547180021872 C 1.94586007917532 N 1.15022738342134 C 1.24064505107964 N 0.40415367237564 C 0.34950836519569 C -0.82310378284313 C -2.16702388087503 H -3.00242303703074 H -2.25741645766201 H -2.28290516906114 C -0.70303739474396 H -0.78039739474396 H -0.78039739474396 H -0.78039739474396 H -0.78039739474396 H -0.76397393644740 H -0.51456948946017 H -3.024284057514484 H -1.51456948946017 H -3.0224242568 H 0.26050022476613 H -0.25757866661 C 2.19245220837908 C 3.00920699963170 C 2.8696324148930 H 3.52085443262974 H 3.73835209380879 H 2.26320881083762 H 2.25157787069680 H 0.79028697062368 C 0.62240176946257 C -0.79569216909177 N -1.37246677911365 C -2.565946118480584 C -5.5654614810029 N -3.20347431735088 C -4.53244460237828 C -5.5696118480544 C -5.579783988647827 C -6.860635361144303 H -7.259423238347180 H -7.25942323847180	1.56802580240128 2.12882896081191 1.03299847920164 -0.05568032826182 -1.0692987303373 -2.11499145868648 -3.33150618030967 -3.42480687503060 -3.444875779354386 -1.34280687503060 -2.38393129481778 -2.27573818803979 -2.36579430886828 -1.30635355770883 -2.365019583223616 -5.61878076699907 -4.78988361670816 -5.61878076699907 -4.88091480593891 -1.737968007279 2.0628012951493 0.202517582235404 -3.46682438762012 -4.17854997694668 -2.0251975822354 0.7343109137578 0.730730734306 1.7633068805230 2.83202732005345 2.659011839633 2.70587104502622 1.56308081531443 2.6590517839633 2.559011389633 2.5590511389633 2.5590517839632 2.65978707938 -1.82936092428320 -1.72300423755914 0.24125780707938 -1.82936092428320 -1.72300423755914	-0.44269212356758 0.90412466839269 1.90567759829530 1.78058231103132 2.69942460224604 2.52706774225047 3.32832443574563 4.34503271854406 3.60019233906069 4.30565620260019 2.85455129205759 2.85455129205759 3.08097507546235 5.38657500861344 6.09314857431308 4.91530140927344 5.97219968586911 5.04625049975621 4.32651377938116 5.58984450210265 5.7739371456792 3.85627670972933 2.62981390096151 1.72878858482180 3.7559469220458 3.84341442578426 3.90391474494738 2.90391474494738 2.90391474494738 2.90391474494738 2.90391474494738 2.90391474494738 1.223048205404 -0.78164512820158 -0.33495310034920 0.66772577339372 0.50409872024737 1.06476276503393 0.11901571602505 -0.35113551395703 -0.95827616676363 0.50158126142185 -0.39414082147717 1.2909987253479 1.80950159688996

C -5.85715404265620 0.43096582468041 -1.09953962225564
H -6.28807080618034 1.39641008721292 -0.79838137645746
H -6.58014381153136 -0.05590503650131 -1.76798095548170
H -4 94730097469878 0 62627850391692 -1 68341219669277
H _4 03325070320164 1 16050785648086 1 43452013027035
II 4 40005576946440 0 42946702005500 1 04772509029061
H -4.40905570840449 -0.45840705005509 1.94772508058001
H -2.545488/3128551 -0.3906169/965095 0.49180008805515
C -3.41707900259293 2.80491030808604 0.00827762561700
C -2.79944374725389 3.95442970667081 -0.43207253571004
C -1.45284537523516 3.92267937992739 -0.83874767872278
H -0.94365849893231 4.81597426594982 -1.19389351443956
H -3 35948382529786 4 88841280306208 -0 46880808344874
H _4.46156538015036 _2.82281081108675 _0.30428404550250
H 0.50000206021660 2.17165002780556 2.20401067247602
II 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
H 1.14321407022833 3.32197283972043 -1.28940200023070
H 3.189/953/9244/4 0.5550/801386114 -0.33561892219650
H 3.21496408406991 1.94157893033602 -1.43879442137857
H 3.28267510073957 -0.26214496821019 -2.65809124689478
H 1.85942062185782 0.66429064704577 -3.12193642780526
O -1.17942238839704 -1.45884770768108 0.34597132558953
H -1.32284563685273 -2.01941875253787 -0.43467897035865
Table S17. Cartesian coordinates (Å) for CSD Refcode YETNIU02
Atom X V Z
$\frac{1}{C_{\rm P}} = 0.18020750050401 = 0.12204061882225 = 0.04565424142504$
$C_{1} = 0.13037750050401 = 0.15204701885525 = 0.04505454142574$
U -1.01/54425850101 -1.45954//995/418 -1.15840015151590
H -1.9801993/1/910/ -1.3423834//23805 -1.2240344131/8/3
N 0.82667709717894 1.19433645980383 1.15021755471634
C 0.84503226240239 2.48563556948678 0.41944832939845
C 1.15706118943619 2.27110572077288 -1.04414665368548
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.23589338491543 -1.79445152915901
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.23589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097
C 1.15706118943619 2.27110572077288 -1.04414663368548 C 1.81399692187291 3.23589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.70659675569160
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.2589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.70659675569160 C 0.98469946976076 0.8168503569450 -2.7576955573241
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.23589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.70659675569160 C 0.98460946976076 0.81683033669450 -2.87679552525241 N 0.73872940662568 1.0930538653347 -1.56500770667718
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.23589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.706596755569160 C 0.98460946976076 0.81683033669450 -2.87679552525241 N 0.73787940662698 1.09305286853247 -1.56620279662719 D 0.500164269234 0.0420567200677 -3.075571675557
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.23589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.70659675569160 C 0.98460946976076 0.81683033669450 -2.87679552525241 N 0.73787940662598 1.09305286853247 -1.56620279662719 N 0.59416546823460 -0.43936767300677 -3.30753716785857
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.23589338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.70659675569160 C 0.98460946976076 0.81683033669450 -2.87679552525241 N 0.73787940662698 1.09305286853247 -1.56620279662719 N 0.59416546823460 -0.43936767300677 -3.30753716785857 C 0.973655749559999 -1.06020740713162 -4.51571752976053
C 1.15706118943619 2.27110572077288 -1.04414665368548 C 1.81399692187291 3.2558338491543 -1.79445152915901 C 2.02373694222846 2.97619940021459 -3.15385302694097 C 1.61254103055567 1.77481444612933 -3.706596755569160 C 0.98460946976076 0.81683033669450 -2.87679552525241 N 0.73787940662698 1.09305286853247 -1.56620279662719 N 0.59416546823460 -0.43936767300677 -3.30753716785857 C 0.9736575495599 -1.06020740713162 4.51571752976053 O 1.60284282863812 -0.46479906052659 -5.37836600916641
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