Supporting information for:

Sulfate-induced large amplitude conformational change in a Solomon link

Cuong Dat Do,^a Dávid Pál,^a Andrey Belyaev,^b Marion Pupier,^a Anniina Kiesilä,^b Elina Kalenius,^b Bartomeu Galmés,^c Antonio Frontera,^c Amalia Poblador-Bahamonde^a and Fabien B. L. Cougnon^{a,b†*}

Corresponding Author fabien.b.l.cougnon@jyu.fi

a. Department of Organic Chemistry, University of Geneva, 30 Quai Ernest-Ansermet 1211 Geneva 4, Switzerland

b. Department of Chemistry, Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014
 JYU, Finland

c. Department de Química, Universitat de les Illes Balears, Carretera de Valldemossa km 7.5, 07122 Palma de Mallorca, Baleares, Spain

[†] Current address: Department of Chemistry, Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 JYU, Finland

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1. Methods and general information

Synthesis. The Solomon link was synthesized according to a published procedure^{S1} and isolated by reversed-phase flash chromatography as a trifluoroacetate salt ($SL^{8+}\cdot 8CF_3CO_2^{-}$). The full characterization of the Solomon link in D₂O can be found in reference S1.

NMR analyses. Spectra were measured using a Bruker Advance III HD-Nanobay 400 MHz spectrometer equipped with a 5-mm Prodigy CryoProbe, or a Bruker Avance III 500 MHz spectrometer equipped with a 5-mm DCH 13 C- 1 H/D helium-cooled cryogenic probe. NMR solvent: CD₃OD (ARMAR Isotopes, Acros Organics). All signals were internally referenced to the solvent residue (CD₃OD: 3.310 ppm).

¹**H NMR titrations.** All the titrations were performed in CD₃OD. Tetrabutylammonium salts were purchased from Fluka (tetrabutylammonium chloride), Acros Organics (tetrabutylammonium bromide, tetrabutylammonium iodide, tetrabutylammonium perchlorate), Sigma-Aldrich (tetrabutylammonium thiocyanate, tetrabutylammonium nitrate, tetrabutylammonium triflate, tetrabutylammonium hexafluorophosphate, tetrabutylammonium perchenate) and Alfa Aesar (tetrabutylammonium sulfate, 50% w/w aq. soln.).

Mass spectrometry. Mass spectrometry experiments were performed on an Agilent 6560 ESI-IM-QTOF mass spectrometer equipped with AJS ESI ion source. Samples were injected using direct infusion from a syringe pump with a flowrate of 5 μ l/min. Nitrogen was used as dry-, sheath and nebulizer gas from nitrogen generator. A dry-gas temperature of 225 ° C, drying gas flow rate of 5 l/min, nebulizer pressure of 30 psi, sheath gas temperature of 225 ° C and sheath gas flow of 10 l/min were used. Capillary voltage of 2000 V and fragmentation voltage of 400 V were set as source parameters. The mass spectrometer was calibrated with an ES tuning mix from Agilent Technologies. Data was acquired with MassHunter Acquisition B.09.00 and analysed using MassHunter Qualitative analysis B.08.00 as software packages from Agilent Technologies, USA.

In IM-MS experiments both He (5.5) and N₂ (5.0) were used as drift gas. Pressures for drift tube and high-pressure funnel were set as 3.95 and 3.70 Torr (3.80 Torr for N₂), respectively. The drift tube entrance and exit voltages for He measurements (values for N₂ in parenthesis) were set as 875 V and 133 V (1574 V and 224 V). A trap filling time of 5000 μ s and trap release time of 350 μ s were used. For multi-field measurements, the drift tube entrance voltage was varied from 563 to 875 V with 52 V increments (1074 V to 1674 V with 100 V increments). ES tuning mix was measured as a quality control sample for the collision cross section (CCS) values.^{\$2,83}

The stock solution of Solomon link was prepared as 0.5 mM in MeOH. The stock solutions of salts were 1, 2 or 5 mM in MeOH. Samples were prepared with 1 μ M host concentration and 1:1 host:guest ratio in methanol. For those experiments, both analytical grade tetrabutylammonium hydrogen sulfate and tetramethylammonium sulfate were used and gave the same results.

Theoretical CCS values were calculated with IMoSSuite 1.12^{S4} by using experimental parameters (gas, temperature, and pressure). Coordinates for the calculations were obtained from DFT calculated structures (see sections 10 and 11). Several theoretical approaches were tested: Project approximation (PA), trajectory method with Lennard-Jones parameters (TMLJ), diatomic trajectory method (DTM), and exact hard sphere scattering (EHSS/DHSS). The number of rotations was 3 with 300 000 gas molecules per rotation in all calculations. The best comparison to experimental data was obtained using TMLJ method with helium gas. EHSS and DTM methods with helium also resulted to similar results (error < 3%).

UV-Vis spectroscopy. UV-Vis spectra were measured using a Perkin Elmer Lambda 650 spectrophotometer (2009) with a 1 nm step rate and standard 10 mm quartz cuvettes. Emission spectra were recorded on a Cary Variant Eclipse spectrofluorimeter (2009) with an excitation wavelength of 400 nm.

High-performance liquid chromatography (HPLC). Chromatograms were obtained from Shimadzu LC-20AT liquid chromatograph equipped with an SPD-M10A VP diode array detector, SCL-10A VP system controller, and DGU-14A degasser. XBridge C18 column (3.5-micrometer diameter particle size, 4.6*150 mm) was used for all analytical experiments. 20 microliter aliquots (0.085 mM) were

injected and eluted with $H_2O/MeCN$ solution (TFA 0.1%) in a gradient mode (5-50% of MeCN) within 30 minutes.

Theoretical methods. The geometries included in this study have been fully optimized (no imaginary frequency) at the BP86-D3/def2-TZVP^{S5,S6} level of theory with the latest available correction for dispersion $(D3)^{S7}$ using the program TURBOMOLE version 7.0.^{S8} In order to reproduce solvent effects, we have used the conductor-like screening model COSMO^{S9} (which is a variant of the dielectric continuum solvation models)^{S10} with the parameters for methanol.



Figure S1. (a) Reidemeister moves allowing the transition between the C_4 - and D_2 -symmetric conformations of the Solomon link. (b) The conformational transformation significantly changes the relative distance between many atoms of the Solomon link. In this figure, we highlight the change in relative distance between protons i and i', or between two protons l located on the same macrocycle. (c) Zoom on one of the two binding sites of conformer **2**. One sulfate anion binds in each binding site *via* the formation of four N-H…O-S and ten C-H…O-S hydrogen bonds.

2. NMR characterization of conformer 1 in CD₃OD



Figure S2. Overlap of the COSY (black) and NOESY (red) spectra of the Solomon link in conformation **1** (0.93 mM in CD₃OD, 298 K, 500 MHz). COSY correlations are highlighted with rectangles. For the NOESY spectrum, $d_8 = 300$ ms. Protons **k** and **l** are particularly upfield shifted because they face the xylylene units in a T-shape relationship.



Figure S3. NOESY spectrum of the Solomon link in conformation **1** (0.93 mM in CD₃OH, 298 K, 500 MHz, $d_8 = 300$ ms). The highlighted NOE correlations were used to determine the conformational state of the acylhydrazone linkages.



Figure S4. ¹³C NMR spectrum of the Solomon link in conformation 1 (0.93 mM in CD₃OD, 298 K, 125 MHz).



Figure S5. HSQC spectrum of the Solomon link in conformation 1 (0.93 mM in CD₃OD, 298 K, 125 MHz).

3. ¹H NMR anion titrations in CD₃OD



Figure S6. ¹H NMR spectra of the Solomon link (0.93 mM in CD₃OD, 298 K, 500 MHz) (a) before and after addition of 2 equiv. of (b) Cl⁻, (c) Br⁻, (d) I⁻, (e) CF₃SO₃⁻, (f) PF₆⁻, (g) SCN⁻, (h) NO₃⁻, (i) ReO₄⁻, (j) ClO₄⁻ and (k) SO₄²⁻. The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively. In cases b-j, the Solomon link remains in conformation **1**. The addition of the anions only results in a shift of the protons g' and a', indicating an interaction between these anions and the NH' located on the external surface of the Solomon link (in conformation **1**). In case k, the addition of SO₄²⁻ results in the appearance of conformer **2**.



Figure S7. ¹H NMR spectra of the Solomon link (0.93 mM in CD₃OD, 298 K, 500 MHz) (a) before and after addition of (b) 1.82 equiv., (c) 2.21 equiv., (d) 2.60 equiv., and (e) 3.38 equiv. of SO_4^{2-} . The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively.

Table S1. Values used for the Hill plot $\log\theta/(1-\theta) = f(\log[SO_4^{2-}])$ and the speciation curve $\theta = f(\log K'[SO_4^{2-}])$	O4 ²⁻])
Values were obtained from the NMR titration of the Solomon link (0.93 mM in CD ₃ OD) with SO4 ²⁻ at 313	K.

log [SO ₄ ²⁻]	log K'[SO4 ²⁻]	$\theta = [2]/[SO_4^{2-}]$	$\theta(1-\theta)$	$\log \theta(1-\theta)$
-3.95	-1.05037	0.012	0.01215	-1.91558
-3.79	-0.89037	0.0245	0.02512	-1.60006
-3.65	-0.75037	0.035	0.03627	-1.44046
-3.49	-0.59037	0.06725	0.0721	-1.14207
-3.35	-0.45037	0.095	0.10497	-0.97892
-3.256	-0.35637	0.117	0.1325	-0.87777
-3.18	-0.28037	0.154	0.18203	-0.73985
-3.1	-0.20037	0.2064	0.26008	-0.58489
-3.05	-0.15037	0.26	0.35135	-0.45426
-2.99	-0.09037	0.3262	0.48412	-0.31505
-2.95	-0.05037	0.37	0.5873	-0.23114
-2.9	0	0.43	0.75439	-0.12241
-2.87	0.02963	0.47	0.88679	-0.05218
-2.84	0.05963	0.5345	1.14823	0.06003
-2.78	0.11963	0.6622	1.96033	0.29233
-2.75	0.14963	0.73	2.7037	0.43196
-2.7	0.20963	0.79	3.7619	0.57541
-2.65	0.27963	0.83	4.88235	0.68863
-2.61	0.32963	0.84	5.25	0.72016
-2.57	0.38963	0.85	5.66667	0.75333
-2.5	0.44963	0.86	6.14286	0.78837



Figure S8. ¹H NMR spectra of the Solomon link (0.85 mM in CD₃OD, 303 K, 500 MHz) (a) before and after addition of (b) 1 equiv. of tetrabutylammonium (+)-camphor-10-sulfonate (TBA(+)CS), (c) 3 equiv. of TBA(+)CS, and (d) 3 equiv. of NaMeSO₃. No conformational switch was observed upon addition of the two alkane sulfonates.

4. NMR characterization of conformer 2 in CD₃OD



Figure S9. Overlap of the COSY (black) and NOESY (red) spectra of the Solomon link in conformation **2** (0.93 mM in CD₃OD with 2.6 equiv. of SO₄^{2–}, 313 K, 500 MHz). COSY correlations are highlighted with rectangles. For the NOESY spectrum, $d_8 = 300$ ms. Protons **b** and **c** are particularly upfield shifted because they face the xylylene units in a T-shape relationship.



Figure S10. NOESY spectrum of the Solomon link in conformation **2** (0.93 mM in CD₃OD with 2.6 equiv. of SO_4^{2-} at 313 K, 500 MHz, $d_8 = 300$ ms). The highlighted NOE correlations were used to determine the conformational state of the acylhydrazone linkages.





Figure S11. ¹³C NMR spectrum of the Solomon link in conformation **2** (0.93 mM in CD₃OD with 2.6 equiv. of SO_4^{2-} , 313 K, 125 MHz).



Figure S12. HSQC spectrum of the Solomon link in conformation **2** (0.93 mM in CD₃OD with 2.6 equiv. of SO_4^{2-} at 313 K, 125 MHz).



5. ESI-MS characterisation of the host-guest complexes

Figure S13. (+)ESI-MS spectra of (a) 1 μ M Solomon link in MeOH and (b) Solomon link + TBAHSO₄ (both 1 μ M, 1:1 ratio) in MeOH. It is interesting to note that sulfate complexes are already present before addition of TBAHSO₄ (profile spectrum a): the Solomon link is able to catch trace amounts of sulfate from the environment, showing its high affinity towards sulfate.



Figure S14. (+)ESI-MS spectrum of the Solomon link with mixed guests TBAHSO₄, TBAClO₄, TBAPF₆, TBACF₃SO₃ and TBAReO₄. All 1 μ M, 1:1:1:1:1 molar ratio in methanol. The inset shows the theoretical (red) and experimental (black) isotopic distribution for [SL+2SO₄]⁴⁺ ion.



Figure S15. (+)ESI-MS spectra of (a) the Solomon link in methanol and the Solomon link with (b) TBAHSO₄, (c) TBAClO₄, (d) TBAReO₄, (e) TBACF₃SO₃ and (f) TBAPF₆ (1 μ M each, 1:1 ratio in methanol). The experimental and theoretical mass accuracies of the peaks are shown in Table S2.

Table S2. Observed ions, their experimental and theoretical m/z values, mass accuracies, drift times and ^{DT}CCS values in N₂ and in He. Drift times and CCS values for ClO₄⁻ complexes could not be resolved from SO₄²⁻ complexes and are therefore not shown in the table.

Ion	$m/z \exp$	m/z theor	$\Delta m/z$	DT in	DTCCS _{N2}	DT in	DTCCS _{He}
[SL- 2H] ⁶⁺	383.8174	383.8151	(mDa) -2.34	15.88		He (ms)	
[SL -3H] ⁵⁺	460.3775	460.3767	-0.8	17.24	626.5	8.54	412.4
[SL -H+SO ₄] ⁵⁺	479.9709	479.9701	-0.8	17.26	629.9	8.55	413.6
[SL -4H] ⁴⁺	575.2190	575.2190	0.0	19.54	568.9	10.09	395.4
[SL -2H+SO ₄] ⁴⁺	599.7112	599.7109	-0.3	19.62	570.9	10.12	401.7
[SL +2SO ₄] ⁴⁺	624.2026	624.2027	0.1	19.32	560.3	9.72	378.8
[SL -3H+PF ₆] ⁴⁺	611.7135	611.712	-1.5	19.73	572.3	10.15	399.6
$[\mathbf{SL} - \mathbf{H} + \mathbf{SO}_4 + \mathbf{PF}_6]^{4+}$	636.2048	636.2038	-1	19.49	562.1	9.83	384.2
$[SL - 2H + 2PF_6]^{4+}$	648.4562	648.4558	-0.4	19.81	571.6	10.15	395
[SL -3H+OTf] ⁴⁺	612.7095	612.709	-0.5	19.85	579.7	10.32	404.9
[SL -H+SO ₄ +OTf] ⁴⁺	637.2026	637.2008	-1.8	19.67	571.6	10.02	387.4
[SL -2H+2OTf] ⁴⁺	650.2004	650.1989	-1.5	20.33	591.1	10.48	410.1
[SL -3H+ClO ₄] ⁴⁺	600.2097	600.2081	-1.6	19.67	573.2	10.16	399
[SL -H+SO ₄ +ClO ₄] ⁴⁺	624.6996	624.6999	0.3				
[SL -2H+2ClO ₄] ⁴⁺	625.1986	625.1972	-1.4				
[SL -3H+ReO ₄] ⁴⁺	637.7056	637.7041	-1.5	19.63	570.0	10.14	396.8
$[\mathbf{SL} - \mathbf{H} + \mathbf{SO}_4 + \mathbf{ReO}_4]^{4+}$	662.1959	662.1960	0.1	19.49	561.8	9.83	384.3
[SL -2H+2ReO ₄] ⁴⁺	701.1905	701.1912	0.7	19.81	574.2	10.15	393.9
[SL -5H] ³⁺	766.6219	766.6229	1.0				
[SL -3H+SO ₄] ³⁺	799.2781	799.2787	0.6				
[SL -H+2SO ₄] ³⁺	831.9337	831.9345	0.8				

6. Variable temperature ¹H NMR in CD₃OD



Figure S16. Variable temperature ¹H NMR spectra of the Solomon link (0.93 mM in CD₃OD, 500 MHz) in the presence of 2.6 equiv. of SO_4^{2-} . The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively.



Figure S17. Variable temperature ¹H NMR spectra of the Solomon link (0.93 mM in CD₃OD, 500 MHz), confirming that no conformational switch occurs in the absence of sulfate.



Figure S18. Variable temperature ¹H NMR spectra of the Solomon link (0.93 mM in CD₃OD, 500 MHz) with (a) 2.6 equiv. TBAReO₄ measured at 298 K and 313 K; and (b) 2.6 equiv. TBAClO₄ measured at 298 K and 313 K. These data show that these anions do not trigger any conformational switch, even at higher temperature.

7. UV-Vis characterisation of conformers 1 and 2 in CH₃OH



Figure S19. Normalized absorption (dashed line) and emission (solid line) spectra of the Solomon link alone (85 μ M in pink) and with 3.0 equiv. of SO₄²⁻ (in blue). Solvent: MeOH. Differences in the absorption spectra reflect differences in packing of the aromatic units in conformers 1 and 2.



Figure S20. (a) UV-Vis spectra and HPLC chromatograms (monitored at 360 nm) of freshly prepared (solid line) and 7 days old (dashed line) solutions of the Solomon link. (b) UV-Vis spectra and HPLC chromatograms (monitored at 360 nm) of freshly prepared (solid line) and 7 days old (dashed line) solutions of the Solomon link with 3.0 equiv. of $SO_4^{2^-}$. These data show that the unbound conformer 1 degrades slightly faster than the sulfate-bound conformer 2 in methanol, suggesting that sulfate stabilizes the Solomon link to some extent and reduces the kinetics of acylhydrazone exchange.





Figure S21. Titration in water. (a) Partial ¹H NMR spectra of the Solomon link (0.93 mM in H₂O/D₂O 95/5, 298 K, 500 MHz) during the titration with SO₄^{2–} (0–1.5 equiv.). The downfield shift of the protons NH', a', g', and k' shows that SO₄^{2–} interacts with the external surface of the Solomon link. (b) Protons NH and NH' were assigned by NOESY (d₈ = 300 ms) after addition of 1.5 equiv. SO₄^{2–}. (c) Variation of the chemical shifts of protons a' (hollow circles) and g' (full circles) as a function of the concentration of SO₄^{2–}. The orange band represents the standard deviation over three titrations. Precipitation of the sample in the course of the titration prevented us to quantitatively assess binding.



Figure S22. ¹H NMR spectra of the Solomon link (0.93 mM in 500 μ L of CD₃CN, 500 MHz) before (green) and after the addition of 3 equiv. of SO₄²⁻ at 302 K (purple) and at 327 K (red).



Figure S23. ¹H NMR spectra of the Solomon link (0.93 mM in 500 μ L of CD₃OD, 298 K, 500 MHz) in the presence of 3 equiv. of SO₄²⁻ (a) before and after addition of (b) 2 μ L, (c) 5 μ L, (d) 10 μ L, (e) 15 μ L, (f) 20 μ L, (g) 25 μ L, (h) 30 μ L, and (i) 40 μ L of D₂O. The signals corresponding to conformers **1** and **2** are coloured in black and blue, respectively. Water highly solvates sulfate and stabilises conformer **1** (see ref. S11). As a result, addition of water disrupts the host-guest complex **2**·**2SO**₄²⁻, and the Solomon link switches back to conformer **1**.

9. Evidence for the Solomon link contraction upon sulfate binding



Figure S24. Overlaid DOSY of the Solomon link (CD₃OD, 313 K, 500 MHz) in conformations **1** (pink colour) and **2** (blue colour). The diffusion coefficients were measured to be $4.15 \cdot 10^{-10} \text{ m}^2 \cdot \text{s}^{-1}$ (**1**) and $4.75 \cdot 10^{-10} \text{ m}^2 \cdot \text{s}^{-1}$ (**2**). ^a Hydrodynamic radii and volumes were calculated using the Stokes-Einstein equation assuming both conformers to be spherical; volumes were also calculated using dimensions from the DFT minimized models for comparison, approximating them as spheres ^b and cylinders ^c.

10. Comparison between the different conformers of the Solomon link



Figure S25. Comparison between the NMR spectra of the three conformers of the Solomon link currently known. Two of these conformers (1 and 2) are described in this article. Conformer **3** has been described elsewhere.^{S11} (a) ¹H NMR spectrum of the Solomon link in conformation **1** (CD₃OD, 298 K, 500 MHz). The Solomon link also adopts this conformation in D₂O.^{S1} (b) ¹H NMR spectrum of the Solomon link in conformation **2** (CD₃OD with 2.6 equiv. of SO₄^{2–}, 313 K, 500 MHz). (c) ¹H NMR spectrum of the Solomon link in conformation **3** (CD₃CN, 298 K, 500 MHz). Key NOE correlations are highlighted with dotted lines.

11. DFT calculations

Table S3 presents a summary of the energies associated with the sulfate-free Solomon link (conformer 1) and the complexes formed with one or two sulfate anions (conformer 2). Despite several attempts, satisfactory models of the intermediate complex formed with one sulfate anion proved particularly difficult to obtain. Figure S26 shows one example of the structures calculated for the complex with one sulfate anion (for the geometry with two sulfate anions, refer to Fig. 1 in the main text). Notably, the formation energy of the Solomon link bound to one sulfate anion is calculated to be -45.8 kcal·mol⁻¹ (excluding entropic effects). The formation energy with two sulfate anions is significantly higher at -138.0 kcal·mol⁻¹, more than twice the energy of the interaction with only one anion.

This substantial difference arises because the introduction of the first sulfate anion incurs an energy cost to transition from conformer 1 to conformer 2. Once this transition occurs, the entry of the second sulfate anion becomes more favourable. Consequently, it is plausible that the complex with only one sulfate anion represents a transient intermediate that has not been experimentally detected.

Table S3. Total energies of the different complexes formed between the Solomon link and sulfate. The formation energies of the complexes are also indicated.

Host-guest complex	E (Hartries)
1 (C ₄ symmetry)	-7472.8905009067
Solomon link + SO_4^{2-} (D ₂ symmetry)	-8172.6045304824
$2 + 2 \text{ SO}_4^{2-}$ (D ₂ symmetry)	-8872.3925662255
Host-guest complex	$\Delta E_{f} (kcal \cdot mol^{-1})$
Solomon link + SO_4^{2-} (D ₂ symmetry)	-45.8
$2 + 2 \text{ SO}_4^{2-}$ (D ₂ symmetry)	-138.0



Figure S26. RI-BP86-D3/def2-TZVP optimized Solomon link bond to one sulfate. The four symmetrically equivalent NH…O H-bonds are indicated as dashed lines. Distances are given in Å.

12. Cartesian coordinates

Con	formation 1	(C ₄ -symmetry)	
С	6.8663452	4.1975156	-2.3501902
C	5 7569916	3 2950359	-2 5031432
G	4 5404070	3.2000000	2.5051452
C	4.5404272	3.7900280	-2.956/526
С	4.3823551	5.1509560	-3.2639092
С	5.4159009	6.0524254	-3.0918206
C	6 6641290	5 5923238	-2 6284339
č	2 0027104	6 1242770	2.0201000
C	3.003/194	0.1342//9	3.3233027
С	2.6544232	5.5201086	3.2405272
С	1.5925581	6.2202085	2.6716909
С	1.7655763	7.6287979	2.4015783
ĉ	2 0640621	0 2002121	2.6112240
C	3.0049031	0.2002131	2.0112240
С	4.1078356	7.4537717	3.1868444
Н	5.2579175	7.1004514	-3.3278829
н	5.0709071	7,9032253	3,4044695
C	0 1005576	E 424010E	0.1011000
C	0.4005570	5.4249105	2.3300222
C	5.8809/11	1.8690526	-2.1/429/9
С	-5.8809711	-1.8690526	-2.1742979
С	-0.4085576	-5.4249105	2.3568222
Ċ	-5 7569916	-3 2950359	-2 5031/32
~	4 5404070	2.2000000	2.0001402
C	-4.5404272	-3./900280	-2.956/526
С	-6.8663452	-4.1975156	-2.3501902
С	-4.3823551	-5.1509560	-3.2639092
C	-6 6641290	-5 5923238	-2 6284339
č	2 6544222	5.5525250 5.5201096	2 2405272
C	-2.0344232	-3.3201088	3.2403272
С	-5.4159009	-6.0524254	-3.0918206
С	-1.5925581	-6.2202085	2.6716909
С	-3.8837194	-6.1342779	3.5235627
л ц	_5 2570175	-7 1004514	-3 3070000
п	-J.2J/J1/J	-7.1004514	-3.3270029
C	-1./655/63	-/.628/9/9	2.4015/83
С	-4.1078356	-7.4537717	3.1868444
С	-3.0649631	-8.2082131	2,6112240
ч	-5 0709071	-7 9032253	3 1011695
~	0.0100011	7.9052255	1 0014055
C	0./1/0/4/	8.4/6264/	1.9/14059
Н	-0.2779376	8.0545412	1.8329235
С	8.1395959	3.7846870	-1.8948917
н	8 3080745	2 7463905	-1 6190714
~	0.3000713	2.7103503	1 0714050
C	-0./1/0/4/	-8.4/6264/	1.9/14059
Н	0.2779376	-8.0545412	1.8329235
С	-8.1395959	-3.7846870	-1.8948917
н	-8 3080745	-2 7463905	-1 6190714
11	2 5262072	4 4600006	2 1720200
п	2.3202973	4.4022220	3.4/29309
Н	4.6760576	5.5626715	4.0061954
Н	3.4295566	5.5040883	-3.6569130
Н	3,7097562	3.0987781	-3.0919125
ч	-2 5262973	-1 1622226	3 1729389
11	2.5202575		1 0001000
н	-4.6/605/6	-5.5626/15	4.0061954
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н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н С	9.9092099 11.1850330 7.9542209 8.1931070 8.4129236 -7.9542209 -8.1931070 -8.4129236 -10.0973628 -9.9092099 -11.1850330 -1.2467135	-3.1897617 -4.5524600 -7.5041580 -7.0008595 -8.5001086 7.5041580 7.0008595 8.5001086 4.6623320 5.1897617 4.5524600 4.8763244	2.0679896 -2.4975539 -3.4415823 -2.5502649 -2.4975539 -3.4415823 -2.5502649 2.1551176 3.0968723 2.0679896 -1.6487523
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Ν	5.	.8782849	0.6346795	1.7400066
С	8.	.4709960	-6.7396550	-1.2909487
С	9.	3057174	-5.6264210	-1.4562741
C C	9. 8	.3057174	-5.6264210	-1.4562741
C C C	9. 8.	.3057174	-5.6264210 -7.1808716	-1.4562741 0.0066291
C C C	9. 8. 9.	.3057174 .1805738 .8266185	-5.6264210 -7.1808716 -4.9621832	-1.4562741 0.0066291 -0.3436494
C C H	9. 8. 9. 9.	.3057174 .1805738 .8266185 .5837628	-5.6264210 -7.1808716 -4.9621832 -5.2923149	-1.4562741 0.0066291 -0.3436494 -2.4576711
C C H C	9. 8. 9. 9. 8.	.3057174 .1805738 .8266185 .5837628 .7016734	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591
С С Н С Н	9. 8. 9. 8. 7.	.3057174 .1805738 .8266185 .5837628 .7016734 .5626553	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518
C C H C H C	9. 8. 9. 8. 7. 9.	.3057174 .1805738 .8266185 .5837628 .7016734 .5626553 .5229487	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434
С С Н С Н С Н	9. 8. 9. 8. 7. 9. 10.	.3057174 .1805738 .8266185 .5837628 .7016734 .5626553 .5229487 .4954043	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257
С С Н С Н С Н С Н	9. 8. 9. 8. 7. 9. 10. 8.	.3057174 .1805738 .8266185 .5837628 .7016734 .5626553 .5229487 .4954043 .4921737	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702
С С С Н С Н С Н С Н С Н С Н	9. 8. 9. 8. 7. 9. 10. 8. 8.	.3057174 1805738 8266185 5837628 .7016734 5626553 5229487 4954043 4921737	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2004087
С С Н С Н С Н С Н С Н С Н	9. 8. 9. 8. 7. 9. 10. 8. -8.	.3057174 1805738 8266185 5837628 .7016734 .5626553 .5229487 .4954043 .4921737 .4709960	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487
СССНСНСНИСС	9. 8. 9. 8. 7. 9. 10. 8. -8. -9.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741
С С С Н С Н С Н С С С	9. 8. 9. 8. 7. 9. 10. 8. -8. -9. -8.	.3057174 1805738 .8266185 5837628 .7016734 5626553 5229487 .4954043 .4921737 .4709960 .3057174 1805738	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291
С С С Н С Н С Н С С С С	9, 8, 9, 8, 7, 9, 10, 8, -8, -9, -8, -9,	.3057174 1805738 .8266185 5837628 .7016734 5626553 5229487 .4954043 .4921737 .4709960 .3057174 1805738 .8266185	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494
СССНСНССССН	9. 8. 9. 9. 10. 8. -8. -9. -9. -9. -9.	.3057174 .1805738 .8266185 .5837628 .7016734 .5626553 .5229487 .4954043 .4921737 .4709960 .3057174 .1805738 .8266185 .5837628	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711
СССНСНСННССССНС	9. 8. 9. 8. 7. 9. 10. 8. -8. -9. -8. -9. -9. -8. -9. -8.	.3057174 1805738 8266185 5837628 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 .7016734	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -0.3436494 1.1178591
СССНСНСННССССНСН	9. 8. 9. 8. 7. 9. 10. 8. -8. -9. -9. -9. -9. -8. -7.	3057174 1805738 8266185 5837628 7016734 5626553 4954043 4921737 4709960 3057174 1805738 8266185 5837628 57016734 5626553	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518
СССНСНСННССССНСНС	9. 8. 9. 8. 7. 9. 10. 8. -8. -9. -9. -9. -8. -7. -7.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.9555434 0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434
СССНСНСННССССНСНСН	9. 8. 9. 8. 7. 9. 10. 8. -9. -8. -9. -9. -8. -7. -9. -10.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.9555434 -0.9555434
СССНСНСННССССНСНСНН	9. 8. 9. 9. 9. 10. 8. -9. -9. -9. -9. -9. -9. -9. -9. -9. -9	3057174 1805738 8266185 5837628 7016734 55225487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.11467027
СССНСНСННССССНСНСНН	9. 8. 9. 9. 9. 9. 10. 8. -9. -9. -9. -9. -9. -10. -8. -8.	3057174 1805738 8266185 5837628 7016734 55229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702
СССНСНСННССССНСНСННН	9. 8. 9. 9. 9. 8. -9. -8. -9. -8. -9. -8. -9. -8. -9. -10. -8. 4.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 57016734 5626553 5229487 4954043 4921737 3614374	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517	$\begin{array}{c} -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ -1.2909487\\ -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ 2.6380025\\ \end{array}$
СССНСНСННССССНСНСНННН	9. 8. 9. 9. 9. 10. 8. -9. -9. -9. -9. -9. -9. -9. -9. -9. -10. -8. -4.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 3614374	$\begin{array}{c} -5.6264210\\ -7.1808716\\ -4.9621832\\ -5.2923149\\ -6.5172853\\ -8.0663429\\ -5.3937554\\ -4.1135067\\ -6.9077457\\ 6.7396550\\ 5.6264210\\ 7.1808716\\ 4.9621832\\ 5.2923149\\ 6.5172853\\ 8.0663429\\ 5.3937554\\ 4.1135067\\ 6.9077457\\ -0.4808517\\ 0.4808517\\ \end{array}$	$\begin{array}{c} -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ -1.2909487\\ -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ 2.6380025\\ 2.6380025\\ 2.6380025\\ \end{array}$
СССНСНСННССССНСНСННННИ	9. 8. 9. 9. 7. 9. 10. 8. -9. -9. -9. -9. -9. -8. -7. -9. -10. -8. -4. -9. -4. -9.	3057174 1805738 8266185 5837628 7016734 55225487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 3614374 3614374 5375539	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 -3.2714589	$\begin{array}{c} -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ -1.2909487\\ -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ 2.6380025\\ 2.6380025\\ 2.2482396\end{array}$
СССНСНСННССССНСНСННННИМ	9. 8. 9. 9. 9. 9. 9. 10. 8. -9. -9. -9. -9. -9. -10. -8. -9. -10. -8. -9. -9. -9. -9. -9. -9. -9. -9. -9. -9	3057174 1805738 8266185 5837628 7016734 55229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 3614374 3614374 5375539	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 -3.2714589 3.2714589	$\begin{array}{c} -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ -1.2909487\\ -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ 2.6380025\\ 2.6380025\\ 2.2482396\\ 2.2482396\end{array}$
СССНСНСННССССНСНСННННИМИ	9. 8. 9. 9. 8. 7. 9. 10. 8. -9. -8. -9. -9. -9. -10. -8. 4. -9. -9. -9. -9. -9. -9. -9. -9. -9. -9	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 3614374 3614374 3614374 5375539 5375539	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 0.4808517 -3.2714589 3.2714589 -7.7213675	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 2.6380025 2.6380025 2.2482396 2.2482396 -2.4206040
СССНСНСННССССНСНСННННИМИМ	9. 8. 9. 9. 8. 7. 9. 10. 8. -9. -8. -9. -8. -9. -8. -9. -10. -8. -4. 9. -9. -9. -6.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626533 4954043 4921737 3614374 3614374 5375539 4768531 4768531	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 -3.2714589 3.2714589 -7.7213675	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 2.6380025 2.6380025 2.2482396 2.2482396 -2.4206040 -2.4206040
СССНСНСННССССНСНСННННИМИМ	9. 8. 9. 9. 9. 10. 8. -9. -9. -9. -9. -9. -9. -10. -8. 4. -9. -9. -10. -8. -9. -10. -8. -9. -10. -8. -9. -6.	3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 3614374 3614374 5375539 5375539 4768531	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 -3.2714589 3.2714589 -7.7213675 7.7213675	$\begin{array}{c} -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ -1.2909487\\ -1.4562741\\ 0.0066291\\ -0.3436494\\ -2.4576711\\ 1.1178591\\ 0.1662518\\ 0.9555434\\ -0.5007257\\ 2.1146702\\ 2.6380025\\ 2.6380025\\ 2.2482396\\ -2.4206040\\ -2.4206040\\ -2.4206040\\ \end{array}$
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СССНСНСННССССНСНСНННИМИМИ ВОННССССССИ	9. 8. 9. 9. 9. 8. -9. -8. -9. -8. -9. -9. -8. -7. -9. -10. -8. -4. -9. -6. omon 6. 7. 6. 2. 3. 3. 4. 4. -2. -2. -2. -2. -2. -2. -2. -2. -2. -2	3057174 18057174 1805738 82266185 5837628 7016734 56226553 5229487 4954043 4921737 4709960 3057174 1805738 8226185 5837628 7016734 5626553 5229487 4954043 4921737 3614374 361446 36146 36165 361	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 0.4808517 0.4808517 -3.2714589 -7.7213675 7.7213675 504 ²⁻ (D ₂ symme 9.0080042 9.2602297 9.9500344 6.1113443 6.8692240 8.2683381 6.1734523 8.9615772 9.014506	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 2.6380025 2.6380025 2.6380025 2.6380025 2.2482396 -2.4206040 -2.4206040 -2.4206040 try) -3.3495359 -4.0157048 2.9207195 -5.7304692 -5.1785052 -5.1532493 -4.7050292 -4.5956463 -5.5504
СССНСНСННССССНСНСННННИМИМ ВСННССССССНС	9. 8. 9. 9. 9. 8. -9. -9. -9. -9. -9. -9. -9. -10. -8. -9. -9. -10. -8. -9. -9. -10. -8. -9. -9. -10. -8. -9. -9. -9. -9. -9. -9. -9. -9. -9. -9	3057174 1805718 8266185 5837628 7016734 5626553 5229487 4954043 4921737 4709960 3057174 1805738 8266185 5837628 7016734 5626553 5229487 4954043 4921737 3614374 361457 361457 361457 361457 361457 361457 361457 371577 3715777 37157777 371577777777777777777777777777777777777	-5.6264210 -7.1808716 -4.9621832 -5.2923149 -6.5172853 -8.0663429 -5.3937554 -4.1135067 -6.9077457 6.7396550 5.6264210 7.1808716 4.9621832 5.2923149 6.5172853 8.0663429 5.3937554 4.1135067 6.9077457 -0.4808517 0.4808517 0.4808517 -3.2714589 3.2714589 3.2714589 -7.7213675 7.7213675 7.7213675 504 ²⁻ (D2 symme 9.0080042 9.2602297 9.950344 6.1113443 6.8692240 8.2683381 6.1734523 8.9615772 8.8314526	-1.4562741 0.0066291 -0.3436494 -2.4576711 1.1178591 0.1662518 0.9555434 -0.5007257 2.1146702 -1.2909487 -1.4562741 0.0066291 -0.3436494 -2.4576711 1.178591 0.1662518 0.9555434 -0.5007257 2.1146702 2.6380025 2.6380025 2.6380025 2.2482396 2.2482396 2.2482396 2.2482396 2.2482396 2.2482396 2.2482396 2.2482396 2.2482396 2.2482396 2.2482395 2.51532493 -4.0157048 -2.9207195 -5.7304692 -5.1785052 -5.1532493 -4.7050292 -4.5956463 -5.5545044
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C H C C N	5.7290199 6.5797424 5.7073000 6.8138492 7.3728199	-6.8636877 -6.2939581 -8.2617002 -9.0080042 -8.1551942	4.1785777 3.8021992 4.0785804 3.3495359 2.2595184
C H C N C	5.7290199 6.5797424 5.7073000 6.8138492 7.3728199 8.6550001	-6.8636877 -6.2939581 -8.2617002 -9.0080042 -8.1551942 -7.7650699	4.1785777 3.8021992 4.0785804 3.3495359 2.2595184 2.3328954
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C H H H	0.8041140 0.4481862 1.9426304 2.7374452	-3.0585918 -2.2418266 -1.7372842 -3.5985883	3.1562999 2.5233110 4.4310555 5.8988688
C H H H	0.8041140 0.4481862 1.9426304 2.7374452	-3.0585918 -2.2418266 -1.7372842 -3.5985883	3.1562999 2.5233110 4.4310555 5.8988688
С Н Н С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040
С Н Н С С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250
С Н Н С С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332
C H H C C H	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332
C H H C C H S	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000
C H H C C H S O	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489
С H H H C C H S O O	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489
С Н Н С С Н S О О	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 0.8549388 0.0000000 0.8674417 0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489
С H H H C C H S O O O	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 -0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489
С Н Н Н С С Н Ѕ О О О	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489
С H H H H C C H S O O O O	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489
С Н Н Н С С Н S О О О О	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 0.8654489
C H H H C C H S O O O O O Conf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 2.8752543 0.8752543 0.8752543	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 0.8654489 0.8654489 0.8654489
C H H C C H S O O O O C	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 0.8674417 -0.8674417 -0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8755556 0.8755556 0.975656 0.975656 0.9756566 0.97566666 0.975666666666666666666666666666666666666	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489 0.8654489 metry) -4.3585100
С Н Н С С Н S О О О О С О С С Я С С Я С И С С Н С С С В С С С С В С С С С С С С С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 0.8674417 -0.8674417 -0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.875556 0.975656 0.975656 0.975666 0.9756666 0.975666666666666666666666666666666666666	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644
С Н Н С С Н S О О О О О С оnf С Н Ч	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.875254556565656565656565656565656565656565	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.300364
С Н Н С С Н S О О О О О С о И Н Н Н В С С С Н Н В С С С Н В С С С С С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 :ormation 2:: 5.0296695 5.5475511 5.4665669	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.875545555555555555555555	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566
С Н Н С С Н S О О О О О С С и Н С С Н Н С С Н Н С С Н Н С С Н В С С С Н В С С С Н С С С С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674414 -0.8674417 -0.8674457 -0.8674457 -0.867457 -0.867457 -0.867457	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8755556 0.87555566 0.97555567 0.97555567 0.97555567 0.97555567	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591
С Н Н С С Н S О О О О О С о С С Я Н Н С С Н Н Н С С Н Н В С С С Н В С С С Я С С С В С С С С С С С С С С С	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 crmation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752545555555555555555555555555555555555	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 0.8654489 0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040
С H H H C C H S O O O O O C H H C C C H C C C C C C C C	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 0.8549388 0.0000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 : 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8755555555555	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 2.126270
С H H H H C C H S O O O O C C H H C C C C	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 Cormation 2:: 5.0296695 5.5475511 5.465569 -0.7138647 0.7439272 1.3375580	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.875555555555	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370
С H H H H C C H S O O O O C Conf C H H C C C C C	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 crmation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 0.8654489 0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287
С H H H H C C H S O O O O Conf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.8674418 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674414 -0.8674414 -0.8674414 -0.8674414 -0.867444 -0.867444 -0.867444 -0.86744 -0.86	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2.804 ²⁻ (D ₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508
С H H H H C C H S O O O O C C H H C C C C C C C	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 formation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 0.8752543 0.87	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489 0.8654489 0.8654489 -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508
С H H H C C H S O O O O Conf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 0.8549388 0.0000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 : ormation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.875444432 0.8752543 0.	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 0.865489000000000000000000000000000000000000
С H H H H C C H S O O O O Conf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 0.8752543 2.504 ²⁻ (D ₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -3.003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123
С H H H C C H S O O O O Conf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.867455 -0.713864 -0.7254573 -0.9312858 -0.7254573 -0.9312858 -0.7254573 -0.9312858 -0.7254573 -0.9312858 -0.7254573 -0.9312858 -0.9	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 0.8752543 0.87	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 0.8654889 0.865489 0.8654889 0.8654888 0.8654888 0.8654888 0.8654888 0.8654889 0.8654888 0.8654889 0.8654889 0.8654889 0.8654889 0.8654889 0.8654889 0.8654889 0.8654889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.8554889 0.85555589 0.8555589 0.8555589 0.8555589 0.8555589 0.8555589 0.8555589 0.8555589 0.8555589 0.8555589 0.8555589 0.85555890000000000000000000000000000000
С н н н н с с н s о о о о о о о о о о о о о о о о о о	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 : : 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.87	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 metry) -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414
С H H H H C C H S O O O O C O n f	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.867457 -0.7138647 -0.7254573 2.9312858 -1.1027651 -3.5320288	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 0.8752543 2.804 ²⁻ (D ₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -0.8654489 0.8654489 -3.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961
С H H H C C H S O O O O Conf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 0.85577000000000000000000000000000000000
Снннсснзоооо Соннссссснснсни	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.7439272 1.337580 1.5484584 2.7189265 -0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 -0.867452	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.077575	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.855100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -2.7751095
С H H H C C H S O O O O С O n f	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 formation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170
Снннсснзоооо Сопf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.7138647 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 0.8752543 2 SO4²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 0.865489000000000000000000000000000000000000
Снннсснзоооо Соннссссснснсннсс	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.7438458 1.027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438927	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2.804²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 0.8654489 -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254
Снннсснзоооо Соnf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.74389272 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.7438997 -0.743897 -0.74457 -0.743897 -0.743897 -0.743897 -0.743897 -0.743897 -0.743897 -0.743897 -0.7457 -0.7457 -0.7457 -0.745	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.750202	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254
СнннССнзОООО Соnf	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 : : 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.875444444444444444444444	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 0.865489 0.86549
Снннсснзоооо Соннссссснснсннсснс	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 : 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.739281 1.7658393 3.8800077	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.03644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315
Снннсснзоооо Соннссссснснснсском	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.743897 -0.5662530 -0.8819620 -0.868250 -0.8819620 -0.8	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.8800077 5.1031***********************************	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -0.8654489 -0.8654489 -3.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.55417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.582157
Снннсснзоооо Соннссссснснснском	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 ormation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.8800077 5.1031889	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.5982157
Снннсснзоооо Соннссссснснсннсснсиси	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.739281 1.7658393 3.8800077 5.1031889 5.2947027	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.303254 -3.7523657 -4.0869315 -3.5982157 -2.2685112
Снннсснзоооо Соннссссснснсннсснспсс	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609 -1.2378609 -1.4860159	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.8800077 5.1031889 5.2947027 6.5793596	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.303644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.55417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.5982157 -4.0869315 -3.5982157 -2.2685112 -1.744460
Снннсснзоооо Ссннссссснснсннсснспссн	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.7438927 -0.743897 -0.5662530 -0.8819629 -1.2378609 -1.2378609 -1.4860159 -1	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.880077 5.1031889 5.2947027 6.5793596 7.4636417	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.5982157 -2.2685112 -1.7444420 -2.3722612
Снннсснзоооо Соннссссснснсннсснсиссна	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609 -1.4392646	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 -0.8752543 0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8746139 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.8800077 5.1031889 5.2947027 6.5793596 7.4636417 -4636417	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 0.8654489 -0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.5782157 -2.2685112 -1.7444460 -2.3723618
Снннсснзоооо С сннссссснснсннсснспсснс	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609 -1.4392646 -1.7982634	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.880077 5.1031889 5.2947027 6.5793596 7.4636417 6.7259313	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 0.8654489 0.8654489 0.8654489 0.8654489 -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5517723 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.5982157 -2.2685112 -1.7444460 -2.3723618 -0.4026173
Снннсснзоооо Соннссссснснсннсснспсснсн	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.0000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 : : 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609 -1.4392646 -1.7982634	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO_4^{2-} (D_2 sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.880077 5.1031889 5.2947027 6.5793596 7.4636417 6.7259313 7.7254794	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -1.855100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.5982157 -2.2685112 -1.7444460 -2.3723618 -0.4026173 -0.0078334
Снннсснзоооо С оннссссснснсннсснсмсснснс	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 Cormation 2:: 5.0296695 5.5475511 5.4665669 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609 -1.4392646 -1.7982634 -1.9820984 -1.9820984 -1.9820984	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.000000 -0.8752543 0.8752543 -0.8752543 0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8752543 -0.8746139 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.8800077 5.1031889 5.2947027 6.5793596 7.4636417 6.7259313 7.7254794 5.6224200	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.000000 0.8654489 -0.8654489 -0.8654489 -0.8654489 0.8654489 -0.8654489 -0.8654489 -0.8654489 -0.8654489 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.5417961 -2.7751095 -6.3759170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.5982157 -2.2685112 -1.7444460 -2.3723618 -0.4026173 -0.007837
Снннсснзоооо С сннссссснснсннсснспсснснс:	0.8041140 0.4481862 1.9426304 2.7374452 0.4592123 -1.0766408 -0.8549388 0.000000 0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.8674417 -0.7138647 0.7439272 1.3375580 1.5484584 2.7189265 0.7254573 2.9312858 1.1027651 3.5320288 3.1647111 3.5435337 -1.1198222 -0.7438997 -0.5662530 -0.6268250 -0.8819629 -1.2378609 -1.4392646 -1.7982634 -1.9820984 -1.8860384	-3.0585918 -2.2418266 -1.7372842 -3.5985883 -4.4009562 -3.7562152 -2.6956921 0.0000000 -0.8752543 0.8752543 0.8752543 0.8752543 2 SO₄²⁻ (D₂ sym 6.8888115 6.6746139 7.8013571 6.2490220 6.6348365 7.4126833 6.1123509 7.5772036 7.8726911 6.2734638 5.5370488 6.9636551 8.1646490 5.8171751 2.8614061 2.7392381 1.7658393 3.880077 5.1031889 5.2947027 6.5793596 7.4636417 6.7259313 7.7254794 5.6224399	3.1562999 2.5233110 4.4310555 5.8988688 2.8811040 0.9951250 1.1544332 0.0000000 0.8654489 -0.8654489 -0.8654489 0.8654489 0.8654489 -0.8654489 -4.3585100 -5.3003644 -3.9469566 -4.5510591 -4.6223040 -3.6176370 -5.6382287 -3.5778508 -2.8418847 -5.5977123 -6.4502414 -4.55177123 -6.4502414 -4.55179170 -1.9807837 -3.3032254 -3.7523657 -4.0869315 -3.5982157 -2.2685112 -2.775108 -2.3723618 -0.4026173 -0.0078334 0.4498105

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H N C C C C C C	2.3015428 2.2406859 2.1813100 1.7772802 1.6775282 1.3453703 1.2378609	-2.2063389 -1.2961017 -3.3496271 -3.1884498 -4.3321606 -4.1407851 -5.2947027	2.7942425 2.2593638 2.0810517 0.8570626 -0.0323444 -1.4194586 -2.2685112
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и н и с с с с с с н н и с н с н с	2.3015428 2.2406859 2.1813100 1.7772802 1.6775282 1.3453703 1.2378609 1.4860159 1.7982634 1.9820984 1.4392646 0.8819629 0.6268250 0.3279072 0.7438997 0.5662530 0.7138647	-2.2063389 -1.2961017 -3.3496271 -3.1884498 -4.3321606 -4.1407851 -5.2947027 -6.5793596 -6.7259313 -7.7254794 -7.4636417 -5.1031889 -3.8800077 -3.8334202 -2.7392381 -1.7658393 -6.2490220	2.7942425 2.2593638 2.0810517 0.8570626 -0.0323444 -1.4194586 -2.2685112 -1.744460 0.4026173 -0.0078334 -2.3723618 -3.5982157 -4.0869315 -5.1301060 -3.3032254 -3.7523657 -4.5510591
"НИССССССННИСНСНС	2.3015428 2.2406859 2.1813100 1.7772802 1.6775282 1.3453703 1.2378609 1.4860159 1.7982634 1.9820984 1.4392646 0.8819629 0.6268250 0.3279072 0.7438997 0.5662530 0.7138647	-2.2063389 -1.2961017 -3.3496271 -3.1884498 -4.3321606 -4.1407851 -5.2947027 -6.5793596 -6.7259313 -7.7254794 -7.4636417 -5.1031889 -3.8800077 -3.8334202 -2.7392381 -1.7658393 -6.2490220 -7.0677000	2.7942425 2.2593638 2.0810517 0.8570626 -0.0323444 -1.4194586 -2.2685112 -1.7444460 -0.4026173 -0.0078334 -2.3723618 -3.5982157 -4.0869315 -5.1301060 -3.3032254 -3.7523657 -4.5510591 -4.2357255
¹ Н N C C C C C C H H N C H C H C H .	2.3015428 2.2406859 2.1813100 1.7772802 1.6775282 1.3453703 1.2378609 1.4860159 1.7982634 1.9820984 1.4392646 0.8819629 0.6268250 0.3279072 0.7438997 0.5662530 0.7138647 1.3650116	-2.2063389 -1.2961017 -3.3496271 -3.1884498 -4.3321606 -4.1407851 -5.2947027 -6.5793596 -6.7259313 -7.7254794 -7.4636417 -5.1031889 -3.8800077 -3.8334202 -2.7392381 -1.7658393 -6.2490220 -7.0677062	2.7942425 2.2593638 2.0810517 0.8570626 -0.0323444 -1.4194586 -2.2685112 -1.7444460 -0.4026173 -0.0078334 -2.3723618 -3.5982157 -4.0869315 -5.1301060 -3.3032254 -3.7523657 -4.5510591 -4.2357257 -4.2357257
"Н И С С С С С С Н Н И С Н С Н С Н Н	2.3015428 2.2406859 2.1813100 1.7772802 1.6775282 1.3453703 1.2378609 1.4860159 1.7982634 1.9820984 1.4392646 0.8819629 0.6268250 0.3279072 0.7438997 0.5662530 0.7138647 1.3650116 1.0921713	-2.2063389 -1.2961017 -3.3496271 -3.1884498 -4.3321606 -4.1407851 -5.2947027 -6.5793596 -6.7259313 -7.7254794 -7.4636417 -5.1031889 -3.8800077 -3.8334202 -2.7392381 -1.7658393 -6.2490220 -7.0677062 -5.8986640	2.7942425 2.2593638 2.0810517 0.8570626 -0.0323444 -1.4194586 2.2685112 -1.7444460 -0.4026173 -0.0078334 -2.3723618 -3.5982157 -4.0869315 -5.1301060 -3.3032254 -3.7523657 -4.5510591 -4.2357257 -5.5177246
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н	-5.4046/04	2.3929850	3.1266429
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Н	-5.5475511	6.6746139	5.3003644

С	-1.3375580	7.4126833	3.6176370
Н	-0.7254573	7.8726911	2.8418847
С	1.1198222	2.8614061	1.9807837
Н	1.2619401	1.9459925	1.4034272
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Н	2.1255648	5.7542870	-1.5049440
С	3.4702255	-1.3811159	-6.2435131
Н	3.6895018	-2.3056962	-6.7775207
Н	4.3880686	-1.7842015	-2.4109969
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Н	5.0685871	-6.2676346	-1.8266930
С	5.2762475	-7.2892060	0.0734835
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H	-1.5038247	-2.1984370	-0.4868995
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S	-3.0439995	0.0000000	0.0000000
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0	3.8784934	1.2335179	0.0202132
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0	2.1403770	0.0041055	-1.2180729
0	-2.1403//0	0.0041055	1.2180/29
SO4 ²⁻	(C1 symmetry)		

S	0.000000	0.0000486	-0.0001021
0	-0.0000001	-0.0001679	1.5178755
0	0.000001	-1.4312497	-0.5057776
0	1.2396160	0.7156845	-0.5059978
0	-1.2396160	0.7156844	-0.5059980

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