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Kinetics and Isotope Effects Study of the Aldol-Tishchenko Reaction Between Lithium Enolates and Aldehydes

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Supporting Information

Kinetics Data

Data Used to determine the order of the aldehyde

	[LiSIBP]	[Benzaldehyde]	Observed Rate
1	1.161e-03	3.00e-02	8.889e-06
2	1.160e-03	7.18e-03	4.716e-07
3	1.160e-03	8.74e-03	7.521e-07
4	1.160e-03	2.25e-02	5.232e-06
5	1.160e-03	1.76e-02	5.198e-06
6	1.160e-03	1.42e-02	2.078e-06
7	1.160e-03	1.06e-02	1.127e-06

Data Used to Determine the order of lithium enolate in the rate law

	[LiSIBP]	[Benzaldehyde]	Observed Rate
1	3.450e-03	1.50e-02	5.031e-06
2	2.384e-03	1.50e-02	3.520e-06
3	1.560e-03	1.50e-02	2.430e-06
4	1.115e-03	1.50e-02	1.972e-06
5	8.340e-04	1.50e-02	1.472e-06
6	5.700e-04	1.50e-02	1.081e-06

Ab Initio Calculations

Geometries and energies are obtained at the HF/6-31++g**. Energies are in atomic units and coordinates are in angstroms. Zero Point Energies are in kcal/mol and given without scaling.

1- Reactions Between Formaldehyde and Lithium Vinyloxyde (LiEn, LiC₂H₃O)

(1) Formaldehyde 6-31++g** HF=-113.87472 ZPE=18.17

O	.000000	.000000	.665113
C	.000000	.000000	-.521030
H	.000000	.928063	-1.097361
H	.000000	-.928063	-1.097361

(2) LiEn from acetaldehyde, η^3 HF =-159.81402 ZPE=31.01

C	1.193917	.151614	-.083386
C	.042736	-.559226	.098565
O	-1.126252	-.128403	-.197285
H	1.220180	.980347	-.780363
H	2.138899	-.227073	.257429
Li	-.625508	1.410817	.463850
H	.107538	-1.512824	.618592

(3) Precomplex LiEn and formaldehyde HF=-273.72075 ZPE(unscaled)=50.98

C	-2.279440	.697524	.165722
C	-1.727968	-.494975	-.186757
O	-.550485	-.885775	.141609
H	-1.857974	1.285785	.970424
H	-3.243112	.992499	-.205066
Li	.041323	.761413	-.228891
H	-2.291288	-1.130664	-.867798
O	1.970757	.745915	-.178437
C	2.438843	-.319087	.117407
H	1.799555	-1.173185	.320820
H	3.518059	-.440557	.184690

(4) TS1 LiEn from acetaldehyde + formaldehyde E(HF)=-273.71203 ZPE=51.82

C	-.563588	1.232117	-.401927
H	-.313298	1.047380	-1.433607
H	-.689280	2.263045	-.114223
C	-1.291475	.271532	.283654
C	1.439209	.535870	.258805
O	-1.351448	-.948790	.003259
Li	.181577	-1.787502	-.363771
H	-1.783737	.587553	1.204597
O	1.546476	-.663665	-.043254
H	1.317779	.827932	1.295033
H	1.858700	1.299121	-.383716

(5) P1 formaldehyde+ LiEn (from acetaldehyde) HF= -273.73798 ZPE=53.78

C	.001105	-1.106461	.362215
H	.014182	-.936248	1.435605
H	-.017713	-2.176365	.175334
C	-1.235997	-.477710	-.192474
C	1.291195	-.440573	-.234706
O	-1.549810	.675614	-.011652
Li	-.047964	1.841797	.264727
H	-1.888405	-1.089322	-.819345
O	1.330924	.886611	-.002286
H	1.323505	-.689075	-1.305510

H	2.125598	-.983725	.221031
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(6) Precomplex Lialdolate + CH₂O, HF=-387.63676 ZPE=73.36

C	1.973320	.582853	.456315
H	1.709545	.467744	1.504105
H	2.938107	1.078001	.388182
C	2.063716	-.780232	-.154265
C	.848942	1.429632	-.225609
O	1.193930	-1.612423	-.082475
Li	-.614845	-.902003	.072850
H	2.965139	-1.029394	-.719451
O	-.358118	.831416	-.131094
H	1.154762	1.609919	-1.266363
H	.885832	2.407227	.267192
C	-2.835962	.330787	-.009837
O	-2.609332	-.840148	.133821
H	-2.949040	.996236	.840453
H	-2.971752	.767274	-.994308

(7) TS2 TS-LiAldolate+Formaldehyde E(HF)=-387.63387 ZPE= 74.39

C	1.840851	-.821688	-.046556
H	2.077809	-1.113573	-1.070758
H	2.583275	-1.306411	.587195
C	2.093920	.655864	.020741
C	.414789	-1.269025	.301164
O	1.257231	1.518039	.080652
Li	-.602444	1.129535	-.307801
H	3.143647	.960340	-.003148
O	-.509430	-.688307	-.522770
H	.239284	-1.030368	1.361090
H	.400063	-2.360277	.235460
C	-2.387789	-.328934	.064761
O	-2.416629	.898688	.145818
H	-2.762040	-.840636	-.812721
H	-2.294705	-.942352	.956018

(8) P2 Product from LiAldolate + Formaldehyde HF= -387.64177 ZPE=76.47

C	1.174171	.802373	.701352
H	.613722	.408575	1.544929
H	1.844539	1.572961	1.068779
C	1.983524	-.324575	.118649
C	.190337	1.412266	-.321038
O	1.504240	-1.333644	-.323795
Li	-.426334	-1.482088	-.476672
H	3.069017	-.211627	.093327
O	-.763312	.507235	-.760334
H	.735971	1.764701	-1.191252
H	-.274349	2.279472	.140539
C	-1.909434	.190227	.154528
O	-1.833547	-1.075001	.498381
H	-1.818573	.904174	.982251
H	-2.781952	.457541	-.443515

(9) TS3; hydride transfer E(HF)=-387.59987 ZPE=75.19

H	.032942	-.317112	1.152608
C	1.302998	-.089437	.594330
C	-1.203888	-.409448	.592987
C	1.006559	1.292372	.046043
H	1.798879	-.097220	1.564622
O	1.569302	-1.032429	-.207198
Li	.305133	-2.057920	-.917483

H	1.814999	1.566725	-.625678
C	-.324593	1.317065	-.707700
O	-1.342993	.874378	.156693
H	-.286938	.700140	-1.597409
H	-.587232	2.324757	-.995793
O	-1.172861	-1.360908	-.233129
H	-1.770779	-.526181	1.510281
H	.968684	2.011011	.858924

(10) p3; Diol Monoester HF=-387.64694 ZPE=76.82

C	-1.447639	-.659996	.530137
H	-1.073539	-.497613	1.539953
H	-2.358042	-1.252892	.623569
C	-1.766826	.716037	-.092222
C	-.463931	-1.519028	-.254456
O	-.722470	1.577323	-.038892
Li	.883563	1.919992	-.345132
H	-2.114268	.539963	-1.122031
H	-2.639907	1.099842	.448556
O	.731109	-.800799	-.617791
H	-.874448	-1.821346	-1.205846
H	-.173725	-2.409748	.295939
C	1.536849	-.403667	.314016
O	2.224728	.572670	.188613
H	1.565581	-1.011815	1.214964

2- Reaction Between Lithium acetate and acetaldehyde

(1) LiAcetate: HF= -198.86078 ZPE=49.61

O	-.538871	-1.110796	-.258361
C	.054399	.018696	-.113173
C	1.542957	-.025946	.130242
C	-.641205	1.202175	-.085948
H	2.018656	-.414798	-.764867
H	1.765498	-.714437	.938743
H	1.957980	.948959	.354742
H	-1.627298	1.249861	-.531729
H	-.156492	2.140479	.104021
Li	-1.794761	-.497750	.793084

(2) Acetaldehyde HF=-152.92779 ZPE= 37.30

O	-1.187489	.392519	.000000
C	.000000	.462435	.000000
C	.920993	-.723966	.000000
H	.490403	1.442991	.000000
H	.354594	-1.645560	.000000
H	1.564478	-.684198	.875039
H	1.564478	-.684198	-.875039

(3) TS1-Me Aldol Rxn LiAcetate + Acetaldehyde HF= -351.80580 ZPE=88.99

C	-.229660	-.805911	.817555
H	.233687	-.358663	1.681302
H	-.228815	-1.882869	.790635
C	-1.323863	-.133645	.265058
C	1.356103	-.041206	-.505878
O	-1.507806	1.103574	.389048
Li	-.077081	2.148250	.166341
C	-2.298524	-.869119	-.625246
O	1.334733	1.202408	-.383003
H	.919169	-.480649	-1.397108
C	2.494085	-.827379	.090035

H	2.702453	-.498277	1.099594
H	3.372977	-.622833	-.519670
H	2.303003	-1.892528	.077645
H	-3.283864	-.812972	-.172928
H	-2.034442	-1.909408	-.768042
H	-2.357185	-.370851	-1.587952

(4) P1-Me LiAldol from LiAcetate + Acetaldehyde HF= -351.83346 ZPE= 90.96

C	.022675	-.652892	.570141
H	.244538	-.318105	1.580405
H	-.039735	-1.736825	.569486
C	-1.303150	-.064969	.170415
C	1.186559	-.149913	-.358158
O	-1.530942	1.123871	.272539
Li	-.001706	2.229090	.077597
C	-2.358178	-.981777	-.384474
O	1.282485	1.198080	-.337557
H	.957350	-.526401	-1.368679
C	2.484964	-.828819	.082755
H	-3.227885	-.419117	-.693453
H	-2.637867	-1.709402	.372259
H	-1.950697	-1.535031	-1.225579
H	2.733184	-.538210	1.100486
H	3.289837	-.494490	-.562853
H	2.426834	-1.915077	.031207

(5) P2-Me LiAldolate + acetaldehyde HF=-504.78287 ZPE=131.98

C	1.071289	.246743	1.020461
H	.567036	-.469148	1.664083
H	1.704132	.865677	1.648105
C	1.925473	-.552836	.057827
C	.000957	1.132877	.335093
O	1.432265	-1.336355	-.717246
Li	-.478946	-1.508655	-.883357
C	3.416531	-.364624	.101409
O	-.922651	.370058	-.371800
C	.608716	2.157997	-.614335
H	-.501959	1.668422	1.137947
C	-2.025388	-.333348	.385015
O	-1.910621	-1.619465	.138338
H	-1.845328	-.060036	1.433367
C	-3.320928	.303093	-.088340
H	3.897619	-.997330	-.630785
H	3.783030	-.603598	1.095837
H	3.658688	.677133	-.088215
H	1.335248	2.784740	-.103435
H	-.174082	2.793293	-1.011087
H	1.095779	1.673579	-1.455635
H	-4.150603	-.168173	.428726
H	-3.441231	.135536	-1.153546
H	-3.343332	1.372543	.107594

(6) TS3-Me HF=-504.73589 ZPE= 130.21 kcal/mol

H	.796382	.439497	-.440358
C	1.185352	-.844123	-.050588
C	-.135555	1.339776	-.031303
C	-.163598	-1.504487	-.301940
C	2.254228	-1.071394	-1.106712
O	1.581916	-.772362	1.157241
Li	1.129240	.573261	2.213306
H	-.141809	-2.478008	.180078
C	-1.320070	-.674005	.262550

O	-1.258047	.610908	-.320529
H	-1.216063	-.582363	1.337897
C	-2.681821	-1.255244	-.065508
O	.126724	1.597784	1.179959
C	.049805	2.434937	-1.058762
H	-.325437	-1.648490	-1.365921
H	2.590700	-2.102947	-1.028981
H	3.102093	-.426465	-.913573
H	1.885305	-.900609	-2.111537
H	-2.818379	-1.329983	-1.139458
H	-3.465599	-.622128	.334685
H	-2.783843	-2.246077	.367097
H	-.716272	3.185089	-.886175
H	-.049909	2.054176	-2.067071
H	1.020325	2.895128	-.926382

X-ray Structure of 4

Notable features of the structure:

1. There is significant disorder in the oxygen positions. Refinement of the occupancies between the two disordered sites on each carbon led to unequal populations. The sum of the occupancies on a given carbon were constrained to 1. No constraints were applied between oxygens on different carbons. Excellent agreement is found between the occupancies of the anti oxygens (occ = 0.571(7) and 0.571(6)) thus proving the anti disposition of the alcohols.

2. There are intermolecular close contacts which indicate hydrogen bonding in chains down the b-axis.

Experimental

Data Collection

A fragment of a colorless blade of C₁₈H₂₂O₂ having approximate dimensions of 0.18 x 0.18 x 0.15 mm was mounted on a quartz capillary using Paratone N hydrocarbon oil. All measurements were made on an Siemens SMART¹⁰ diffractometer with graphite monochromated Mo-K α radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the measured positions of 2993 reflections with $I > 10\sigma$ in the range $3.00 < 2\theta < 45.00^\circ$ corresponded to a primitive monoclinic cell with dimensions:

$$\begin{aligned} a &= 14.2531(12) \text{ \AA} \\ b &= 6.0951(5) \text{ \AA} \quad \beta = 100.711(1)^\circ \\ c &= 17.2394(15) \text{ \AA} \\ V &= 1471.56(37) \text{ \AA}^3 \end{aligned}$$

For $Z = 4$ and F.W. = 270.37, the calculated density is 1.22 g/cm³. The systematic absences of:

$$h0l \neq 2n$$

$$0k0: k \neq 2n$$

uniquely determine the space group to be: P2₁/n (#14)

The data were collected at a temperature of $-85 \pm 2^\circ\text{C}$. Area detector frames were collected using ω scans of 0.3° and a total measuring time of 20 seconds each.

Data Reduction

Data were integrated using SAINT¹¹ with box parameters of $1.6 \times 1.6 \times 0.6^\circ$ to a maximum 2θ value of 46.5° . The data were corrected for Lorentz and polarization effects. No decay correction was necessary.

Analysis of the redundant and equivalent reflections with XPREP¹² indicated that no absorption correction was needed. Of the 6207 reflections which were collected, 2346 were unique ($R_{\text{int}} = 0.035$); equivalent reflections were merged.

Structure Solution and Refinement

The structure was solved by direct methods¹ and expanded using Fourier techniques.² The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement³ was based on 1382 observed reflections ($I > 3.00\sigma(I)$) and 201 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \sum ||F_O| - |F_C|| / |F_O| = 0.060$$

$$R_w = [(\sum w (|F_O| - |F_C|)^2 / \sum w F_O^2)]^{1/2} = 0.079$$

The standard deviation of an observation of unit weight⁴ was 2.73. The weighting scheme was based on counting statistics and included a factor ($p = 0.030$) to downweight the intense reflections. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.29 and -0.30 e-/Å³, respectively.

Neutral atom scattering factors were taken from Cromer and Waber.⁵ Anomalous dispersion effects were included in Fcalc;⁶ the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley.⁷ The values for the mass attenuation coefficients are those of Creagh and Hubbel.⁸ All calculations were performed using the teXsan⁹ crystallographic software package of Molecular Structure Corporation.

References

- (1) SIR92: Altomare, A., Burla, M.C., Camalli, M., Cascarano, M., Giacovazzo, C., Guagliardi, A., Polidori, G. (1994). *J. Appl. Cryst.*, in preparation.
- (2) DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
- (3) Least-Squares: Function minimized: $\sum w(|F_O| - |F_C|)^2$
where $w = 1/\sigma^2(F_O) = 4F_O^2/\sigma^2(F_O^2)$
- (4) Standard deviation of an observation of unit weight:
 $[\sum w(|F_O| - |F_C|)^2 / (N_O - N_V)]^{1/2}$ where: N_O = number of observations; N_V = number of variables
- (5) Cromer, D. T.; Waber, J. T. "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).
- (6) Ibers, J. A.; Hamilton, W. C. *Acta Crystallogr.* **1964**, *17*, 781.
- (7) Creagh, D. C.; McAuley, W.J. "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
- (8) Creagh, D. C.; Hubbell, J.H. "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
- (9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

(10) SMART Area-Detector Software Package; Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(11) SAINT: SAX Area-Detector Integration Program; V4.024; Siemens Industrial Automation, Inc.: Madison, WI, (1995)

(12) XPREP (v 5.03) Part of the SHELXTL Crystal Structure Determination Package; Siemens Industrial Automation, Inc.: Madison, WI, (1995)

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	Cl ₈ H ₂₂ O ₂
Formula Weight	270.37
Crystal Color, Habit	colorless, blade
Crystal Dimensions	0.18x0.18x0.15 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2 θ range)	2993 (3.0 - 45.0°)
Lattice Parameters	a = 14.2531(12) Å b = 6.0951(5) Å c = 17.2394(15) Å β = 100.711(1)° V = 1471.56(37) Å ³

Space Group P2₁/n (#14)

Z value 4

D_{calc} 1.220 g/cm³

F₀₀₀ 584.00

μ (MoK α) 0.78 cm⁻¹

B. Intensity Measurements

Diffractometer Siemens SMART

Radiation MoK α (λ = 0.71069 Å)
graphite monochromated

Crystal to Detector Distance 60 mm

Temperature	-85 °C
Scan Type	ω (0.3° per frame)
Scan Rate	20 seconds per frame
No. of Reflections Measured	Total: 6207 Unique: 2346 ($R_{\text{int}} = 0.035$)
Corrections	Lorentz-polarization

C. Structure Solution and Refinement

Structure Solution	Direct methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(F_o - F_c)^2$
Least Squares Weights	$1/\sigma^2(F_o) = 4F_o^2/\sigma^2(F_o^2)$
p-factor	0.030
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 3.00\sigma(I)$)	1382
No. Variables	201
Reflection/Parameter Ratio	6.88
Residuals: R; R_w ; R_{all}	0.060; 0.079; 0.091
Goodness of Fit Indicator	2.73
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.29 e-/Å ³
Minimum peak in Final Diff. Map	0.30 e-/Å ³

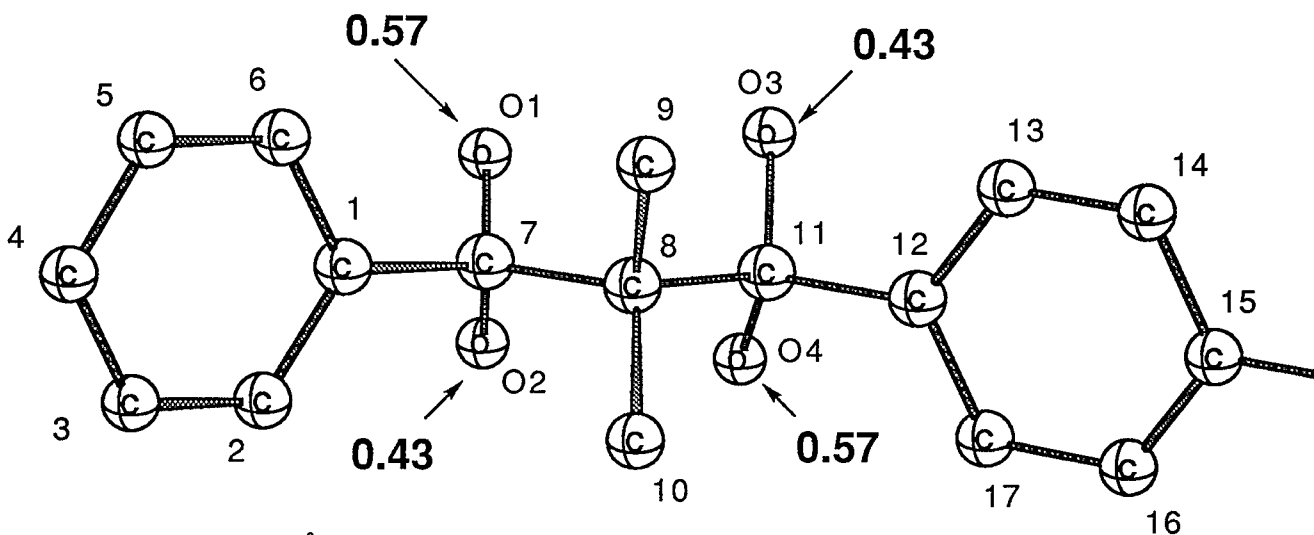
Positional parameters and B(eq) for diol

atom	x	y	z	B(eq)	
O(1)	1.06339(33)	0.26877(77)	0.50276(26)	3.9(2)	(occupancy = 0.571)
O(2)	1.09520(43)	0.0097(10)	0.54696(39)	4.0(3)	(occupancy = 0.429)
O(3)	0.92964(38)	0.30802(95)	0.56192(34)	3.4(3)	(occupancy = 0.429)
O(4)	0.95793(33)	0.00208(73)	0.62600(28)	3.9(2)	(occupancy = 0.571)
C(1)	1.22717(29)	0.23650(68)	0.57308(22)	3.5(2)	
C(2)	1.29315(31)	0.07470(64)	0.60320(23)	3.7(2)	
C(3)	1.39007(34)	0.10566(74)	0.60778(26)	4.5(2)	
C(4)	1.42523(32)	0.29680(84)	0.58155(27)	4.6(2)	
C(5)	1.35955(36)	0.45721(78)	0.54937(27)	4.8(2)	
C(6)	1.26446(33)	0.42914(70)	0.54600(23)	4.0(2)	

C(7)	1.12210(33)	0.20400(71)	0.57136(23)	4.1(2)
C(8)	1.08534(26)	0.28355(60)	0.64600(22)	3.0(2)
C(9)	1.10140(28)	0.53112(64)	0.65693(24)	3.6(2)
C(10)	1.14239(28)	0.16503(65)	0.71945(22)	3.5(2)
C(11)	0.97776(27)	0.23199(62)	0.63598(23)	3.2(2)
C(12)	0.93221(26)	0.31084(64)	0.70316(24)	3.2(2)
C(13)	0.88818(29)	0.51658(66)	0.70033(25)	3.7(2)
C(14)	0.84589(29)	0.58963(64)	0.76187(27)	3.8(2)
C(15)	0.84472(26)	0.46435(69)	0.82799(26)	3.7(2)
C(16)	0.88950(30)	0.25624(70)	0.83096(25)	3.9(2)
C(17)	0.93009(27)	0.18422(64)	0.76979(25)	3.3(2)
C(18)	0.80132(34)	0.54082(83)	0.89377(29)	5.2(2)
H(1)	1.2710	-0.0599	0.6210	4.2
H(2)	1.4332	-0.0068	0.6294	5.3
H(3)	1.4919	0.3186	0.5852	5.7
H(4)	1.3819	0.5887	0.5294	5.5
H(5)	1.2219	0.5431	0.5247	4.5
H(6)	1.1676	0.5624	0.6625	4.2
H(7)	1.0674	0.6063	0.6121	4.2
H(8)	1.0792	0.5780	0.7029	4.2
H(9)	1.1331	0.0111	0.7137	3.9
H(10)	1.2084	0.1977	0.7242	3.9
H(11)	1.1207	0.2136	0.7654	3.9
H(12)	0.8873	0.6079	0.6555	4.3
H(13)	0.8168	0.7305	0.7582	4.5
H(14)	0.8913	0.1656	0.8761	4.9
H(15)	0.9579	0.0421	0.7730	3.8
H(16)	0.8324	0.6712	0.9151	5.8
H(17)	0.7355	0.5699	0.8753	5.8
H(18)	0.8080	0.4309	0.9335	5.8

U values for diol

atom	U11	U22	U33	U12	U13	U23
O(1)	0.0542(32)	0.0476(32)	0.0376(31)	-0.0030(25)	-0.0144(22)	0.0133(24)
O(2)	0.0526(43)	0.0335(41)	0.0649(49)	-0.0131(32)	0.0055(34)	-0.0156(34)
O(3)	0.0356(36)	0.0434(41)	0.0444(41)	0.0040(31)	-0.0038(28)	0.0107(31)
O(4)	0.0568(32)	0.0298(28)	0.0558(33)	-0.0031(24)	-0.0034(24)	-0.0054(25)
C(1)	0.0555(26)	0.0463(26)	0.0258(21)	-0.0016(23)	-0.0029(17)	-0.0033(20)
C(2)	0.0604(30)	0.0370(24)	0.0409(24)	0.0067(23)	0.0061(20)	0.0037(21)
C(3)	0.0646(32)	0.0537(30)	0.0525(28)	0.0138(26)	0.0112(24)	0.0057(25)
C(4)	0.0526(27)	0.0670(33)	0.0533(29)	0.0026(28)	0.0074(22)	-0.0001(26)
C(5)	0.0706(35)	0.0612(32)	0.0531(28)	-0.0111(29)	0.0195(24)	0.0002(26)
C(6)	0.0740(34)	0.0407(27)	0.0343(23)	0.0080(25)	-0.0005(22)	0.0057(20)
C(7)	0.0723(31)	0.0487(30)	0.0307(23)	0.0049(26)	-0.0050(21)	-0.0100(22)
C(8)	0.0432(24)	0.0275(22)	0.0354(22)	0.0037(18)	-0.0095(17)	0.0014(18)
C(9)	0.0519(25)	0.0332(25)	0.0484(24)	-0.0005(19)	-0.0003(19)	-0.0027(19)
C(10)	0.0501(25)	0.0407(24)	0.0361(23)	0.0064(20)	-0.0057(19)	-0.0005(19)
C(11)	0.0450(25)	0.0303(22)	0.0404(23)	0.0005(19)	-0.0060(18)	0.0009(19)
C(12)	0.0301(20)	0.0311(23)	0.0532(27)	-0.0040(19)	-0.0083(18)	0.0029(19)
C(13)	0.0519(26)	0.0353(25)	0.0489(27)	0.0034(22)	-0.0033(21)	0.0057(21)
C(14)	0.0439(25)	0.0333(22)	0.0613(29)	0.0025(20)	-0.0017(21)	0.0045(23)
C(15)	0.0327(23)	0.0482(28)	0.0578(28)	-0.0052(21)	0.0060(20)	-0.0062(24)
C(16)	0.0462(25)	0.0444(27)	0.0556(29)	-0.0030(22)	0.0000(21)	0.0108(24)
C(17)	0.0357(22)	0.0323(22)	0.0533(27)	-0.0015(18)	-0.0015(20)	0.0003(21)
C(18)	0.0561(29)	0.0732(35)	0.0712(33)	0.0031(27)	0.0167(24)	-0.0008(30)



Cartesian Coordinates, Å

O1	13.5458	1.6382	8.5163
O2	13.8576	0.0589	9.2650
O3	11.4498	1.8774	9.5184
O4	11.6478	0.0127	10.6038
C1	15.6548	1.4415	9.7074
C2	16.4988	0.4553	10.2176
C3	17.8654	0.6440	10.2952
C4	18.4506	1.8090	9.8509
C5	17.6176	2.7868	9.3058

C6	16.2731	2.6157	9.2487
C7	14.1627	1.2434	9.6783
C8	13.3997	1.7283	10.9426
C9	13.5936	3.2372	11.1277
C10	13.9775	1.0058	12.1868
C11	11.8984	1.4140	10.7730
C12	11.0339	1.8946	11.9108
C13	10.4155	3.1486	11.8630
C14	9.6155	3.5938	12.9053
C15	9.3870	2.8303	14.0254
C16	10.0157	1.5618	14.0756
C17	10.7902	1.1228	13.0395
C18	8.5577	3.2964	15.1396
H1	16.1258	-0.3650	10.5185
H2	18.4109	-0.0416	10.6619
H3	19.3889	1.9422	9.9132
H4	17.9999	3.5882	8.9679
H5	15.7344	3.3103	8.8882
H6	14.5193	3.4281	11.2228
H7	13.2520	3.6957	10.3690
H8	13.1296	3.5229	11.9059
H9	13.8628	0.0678	12.0900
H10	14.9028	1.2052	12.2675
H11	13.5206	1.3019	12.9654
H12	10.5459	3.7050	11.1039
H13	9.2132	4.4523	12.8428
H14	9.8970	1.0092	14.8395
H15	11.1769	0.2569	13.0931
H16	8.9318	4.0910	15.5016
H17	7.6785	3.4735	14.8272
H18	8.5260	2.6262	15.8123

10|F|o vs 10|F|c for diol

k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF	h	k	l	Fo	Fc	sigF
0	4	501	535	11	0	3	9	67	65	2	1	-5	-1	153	151	4	1	-2	10	47	42	3	1	1	9	46	47	3
0	6	405	416	7	0	3	10	148	149	3	1	-5	0	94	87	5	1	-2	11	21	9	4*	1	1	10	173	167	4
0	8	107	104	2	0	3	11	11	19	12*	1	-5	3	102	103	2	1	-2	13	53	60	8	1	1	11	27	43	5*
0	10	109	105	2	0	3	12	168	165	5	1	-5	5	119	112	3	1	-2	14	40	31	7*	1	1	12	167	176	4
0	12	13	20	13*	0	3	15	18	12	15*	1	-5	6	372	378	7	1	-2	15	7	15	10*	1	1	14	70	51	5
0	14	123	135	2	0	3	16	242	240	4	1	-5	7	0	19	10*	1	-2	16	21	2	14*	1	1	16	57	50	7
0	16	8	5	7*	0	4	-15	0	34	9*	1	-5	8	138	139	4	1	-2	17	104	109	4	1	1	17	43	55	15*
0	18	81	77	6	0	4	-13	77	82	6	1	-5	10	38	29	5	1	-1	-16	105	108	3	1	2	-18	31	35	18*
1	-18	0	9	10*	0	4	-12	44	37	12*	1	-5	11	16	6	17*	1	-1	-14	42	26	4	1	2	-17	120	127	6
1	-17	82	80	7	0	4	-11	74	76	3	1	-4	-14	32	9	7*	1	-1	-11	101	100	3	1	2	-16	68	70	6
1	-15	97	90	5	0	4	-9	45	39	8*	1	-4	-13	26	41	6*	1	-1	-10	88	85	3	1	2	-12	69	72	3
1	-11	105	100	2	0	4	-8	95	94	5	1	-4	-12	113	113	5	1	-1	-9	186	187	3	1	2	-11	80	82	3
1	-10	21	8	5*	0	4	-5	154	163	3	1	-4	-11	206	209	8	1	-1	-8	351	336	6	1	2	-10	286	273	8
1	-5	613	621	14	0	4	-4	171	164	4	1	-4	-9	94	102	3	1	-1	-7	376	381	6	1	2	-7	98	109	5
1	-2	1099	1099	20	0	4	-3	67	75	7	1	-4	-7	120	117	3	1	-1	-6	284	278	5	1	2	-6	5	11	7*
1	1	151	134	5	0	4	0	513	487	9	1	-4	-6	21	3	9*	1	-1	-4	105	116	4	1	2	0	77	69	3
1	3	336	323	8	0	4	1	113	115	6	1	-4	0	104	101	7	1	-1	-3	109	117	5	1	2	1	96	91	2
1	4	705	694	11	0	4	2	66	65	1	1	-4	1	274	273	5	1	-1	-2	168	146	3	1	2	2	55	41	4
1	6	127	104	4	0	4	6	186	189	4	1	-4	4	308	297	8	1	-1	2	605	634	11	1	2	3	186	184	6
1	7	110	96	4	0	4	7	85	89	5	1	-4	6	247	252	4	1	-1	3	243	276	4	1	2	7	241	237	6
1	8	284	297	7	0	4	10	90	88	7	1	-4	7	99	99	5	1	-1	13	23	30	7*	1	2	9	194	197	6
1	9	347	356	9	0	4	14	99	102	14	1	-4	10	73	74	2	1	-1	15	88	86	5	1	2	12	7	3	10*
1	12	166	170	4	0	5	-12	30	40	6*	1	-4	13	39	46	3	1	-1	18	14	2	12*	1	3	-17	30	5	10*
1	13	45	31	3	0	5	-11	28	35	15*	1	-4	14	56	61	4	1	0	-19	34	20	4	1	3	-16	89	93	5
1	14	65	67	4	0	5	-9	98	103	3	1	-3	-14	55	42	7	1	0	-17	156	144	3	1	3	-15	43	55	3
1	16	159	161	4	0	5	-7	49	49	13*	1	-3	-13	233	244	6	1	0	-15	378	362	7	1	3	-11	79	78	2
2	-18	59	63	5	0	5	-6	39	52	3	1	-3	-12	45	48	7	1	0	-13	64	66	2	1	3	-9	100	94	4
2	-17	29	36	7*	0	5	-3	99	100	4	1	-3	-10	29	39	9*	1	0	-11	226	222	4	1	3	-8	86	78	2
2	-15	25	31	14*	0	5	-2	61	54	9	1	-3	-7	19	39	9*	1	0	-9	46	37	4	1	3	-6	17	6	10*
2	-14	308	309	5	0	5	-1	23	29	9*	1	-3	-5	107	106	2	1	0	-7	329	324	5	1	3	1	473	459	8
2	-13	72	75	4	0	5	4	254	245	5	1	-3	-4	47	36	2	1	0	-5	874	868	14	1	3	3	50	38	5
2	-12	207	205	6	0	5	5	84	81	3	1	-3	-3	194	196	4	1	0	-3	763	741	13	1	3	4	36	30	4
2	-2	22	17	4	0	5	8	22	10	4*	1	-3	-2	16	2	5*	1	0	1	452	365	8	1	3	7	18	16	5*
2	0	49	42	4	0	5	10	54	59	16*	1	-3	-1	440	431	9	1	0	3	1271	1326	53	1	3	8	0	6	12*
2	1	498	521	8	0	6	-5	0	5	12*	1	-3	0	53	58	5	1	0	5	158	135	3	1	3	10	31	40	6*
2	3	179	163	3	0	6	-3	13	15	11*	1	-3	2	438	436	7	1	0	7	178	170	6	1	3	11	18	3	12*
2	4	148	151	3	0	6	-2	94	93	2	1	-3	5	75	79	2	1	0	9	8	16	8*	1	3	12	151	155	5
2	5	28	26	3	0	6	-1	14	4	16*	1	-3	6	138	133	5	1	0	11	81	87	3	1	3	13	130	130	7
2	6	92	98	4	0	6	0	35	24	5	1	-3	9	73	86	3	1	0	13	171	166	3	1	3	16	13	8	12*
2	7	485	473	8	0	6	4	61	59	4	1	-3	14	21	13	9*	1	0	15	206	221	7	1	4	-15	110	120	5
2	8	22	14	4*	0	6	6	0	1	19*	1	-3	15	64	66	9	1	0	17	54	41	4	1	4	-10	18	22	16*
2	9	33	29	8*	0	6	7	61	61	3	1	-2	-15	189	192	5	1	1	-18	11	1	13*	1	4	-8	0	8	11*
2	10	20	0	9*	0	6	8	63	57	4	1	-2	-14	28	32	3	1	1	-17	20	27	12*	1	4	-5	94	89	4
2	11	93	93	7	1	-6	-5	0	10	8*	1	-2	-13	42	36	10*	1	1	-15	74	64	8	1	4	-4	21	7	4*
2	16	42	46	5	1	-6	-4	51	39	5	1	-2	-9	136	137	2	1	1	-13	281	286	5	1	4	-3	20	16	8*
3	-14	0	9	10*	1	-6	-2	88	83	12	1	-2	-8	166	165	5	1	1	-12	30	36	5*	1	4	-2	87	84	3
3	-13	23	25	13*	1	-6	-1	20	32	5*	1	-2	-5	22	37	4*	1	1	-5	20	7	8*	1	4	-1	162	164	3
3	-8	100	100	7	1	-6	0	0	1	7*	1	-2	-4	233	216	4	1	1	-1	21	9	4*	1	4	2	29	46	11*
3	-7	62	72	3	1	-6	4	7	28	15*	1	-2	-3	137	133	2	1	1	0	245	303	7	1	4	3	128	128	2
3	1	184	153	3	1	-6	6	15	3	10*	1	-2	-2	61	59	3	1	1	1	1355	1380	36	1	4	5	156	163	5
3	2	165	137	3	1	-6	7	74	71	8	1	-2	-1	339	361	8	1	1	4	285	333	5	1	4	8	204	206	8
3	3	59	57	4	1	-6	8	8	23	7*	1	-2	4	142	124	4	1	1	5	197	188	5	1	4	9	41	35	3
3	4	125	120	2	1	-5	-8	16	29	6*	1	-2	5	7	5	7*	1	1	6	196	184	6	1	4	11	56	52	3
3	5	99	94	3	1	-5	-7	65	68	2	1	-2	6	23	42	2	1	1	7	11	4	8*	1	4	12	51	58	4
3	6	41	25	4	1	-5	-3	38	32	3	1	-2	8	39	44	3	1	1	8	361	356	11	1	5	-12	62	67	10*
5	-11	62	59	3	2	-4	14	31	31	5* 2	2	-1	17	23	4													

k	l	Fo	Fc	sigFh	k	l	Fo	Fc	sigFh	k	l	Fo	Fc	sigFh	k	l	Fo	Fc	sigFh	k	l	Fo	Fc	sigFh				
5	-9	151	150	3	2	-3	-9	104	103	3	2	0	-18	14	17	13*	2	3	-11	0	4	12*	3	-6	-1	61	62	5
5	-6	11	12	14*	2	-3	-8	18	15	12*	2	0	-16	18	3	8*	2	3	-4	209	198	4	3	-6	0	28	34	5*
5	-5	103	113	9	2	-3	-7	40	39	5	2	0	-14	444	435	8	2	3	-3	12	4	6*	3	-6	1	48	43	6
5	-4	8	18	13*	2	-3	-6	97	113	4	2	0	-12	265	289	5	2	3	-2	7	0	7*	3	-6	4	38	27	3
5	-2	7	4	12*	2	-3	-5	30	23	2	2	0	-10	93	84	6	2	3	-1	165	153	4	3	-6	5	56	55	7
5	1	98	98	6	2	-3	0	152	157	3	2	0	-8	385	384	7	2	3	6	18	23	8*	3	-6	7	0	14	9*
5	2	62	58	8	2	-3	1	216	204	4	2	0	-6	480	480	8	2	3	7	182	192	3	3	-5	-11	0	5	17*
5	4	43	39	2	2	-3	2	487	494	12	2	0	-4	656	696	13	2	3	8	53	45	5	3	-5	-8	119	114	3
5	9	51	59	3	2	-3	3	40	48	5	2	0	-2	14	39	2	2	3	10	103	107	5	3	-5	-7	103	109	7
5	12	57	58	4	2	-3	4	117	120	6	2	0	0	292	207	9	2	3	11	141	145	3	3	-5	-6	282	286	5
6	-8	59	64	3	2	-3	5	53	64	5	2	0	2	541	642	15	2	3	12	31	19	10*	3	-5	-4	113	113	3
6	-7	69	65	5	2	-3	9	65	58	3	2	0	4	490	469	9	2	3	13	0	2	10*	3	-5	-3	39	30	11*
6	-6	36	35	3	2	-2	-15	67	64	6	2	0	6	248	246	4	2	3	14	17	6	12*	3	-5	-2	57	63	2
6	-3	151	157	3	2	-2	-12	47	54	7	2	0	8	25	19	4	2	3	15	132	131	11	3	-5	0	49	45	6
6	1	59	62	4	2	-2	-10	84	80	3	2	0	10	34	57	9*	2	3	16	19	17	10*	3	-5	1	67	71	3
6	2	47	42	5	2	-2	-8	14	26	8*	2	0	12	206	216	4	2	4	-14	79	71	7	3	-5	2	32	39	9*
6	3	34	37	8*	2	-2	-7	499	500	8	2	0	14	83	96	3	2	4	-12	31	42	4	3	-5	3	28	31	3
6	5	30	33	19*	2	-2	-5	160	159	4	2	0	16	93	84	7	2	4	-9	53	48	3	3	-5	6	66	72	4
-6	-8	60	54	9	2	-2	-4	45	45	5	2	0	18	115	118	4	2	4	-8	243	249	4	3	-5	8	137	136	3
-6	-7	124	109	4	2	-2	2	61	76	4	2	1	-18	0	5	11*	2	4	-7	79	80	9	3	-5	9	41	43	14*
-6	-6	106	98	4	2	-2	3	64	59	4	2	1	-15	14	4	10*	2	4	-3	22	9	8*	3	-5	10	27	19	10*
-6	-5	56	43	4	2	-2	4	20	45	3	2	1	-11	201	194	6	2	4	-1	111	108	3	3	-5	11	103	98	3
-6	-2	0	10	10*	2	-2	6	59	29	4	2	1	-8	25	7	7*	2	4	0	169	170	6	3	-4	-13	16	8	11*
-6	1	59	60	7	2	-2	7	255	225	7	2	1	-1	295	277	5	2	4	1	19	15	8*	3	-4	-8	293	292	5
-6	2	26	14	11*	2	-2	9	125	123	6	2	1	2	209	192	6	2	4	6	189	184	3	3	-4	-7	138	145	8
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