

Supporting Information for:

Intramolecular cycloaddition of azomethine ylides, from imines of *O*-acetylsalicylic aldehyde and ethyl diazoacetate, to ester carbonyl – experimental and a DFT computational study

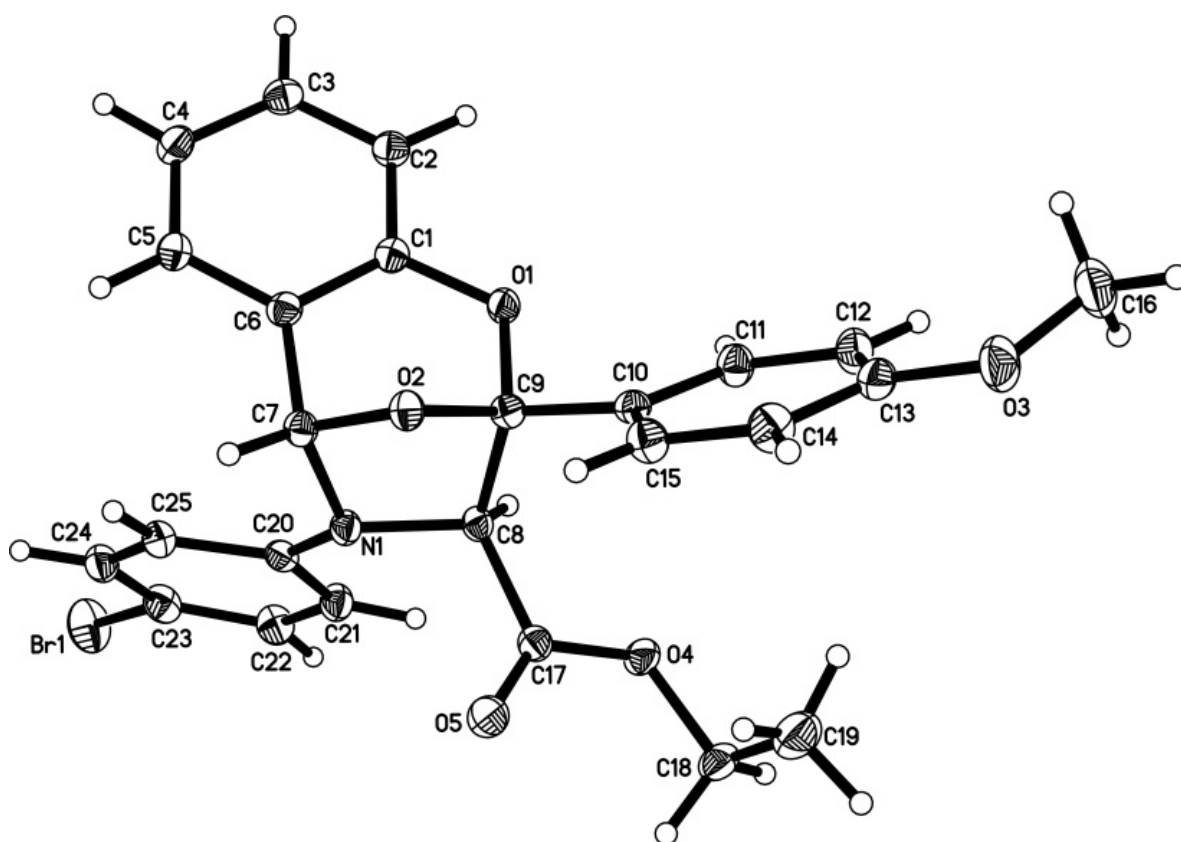
Anastasia P. Kadina,^a Alexander F. Khlebnikov,^{a*} Mikhail S. Novikov,^a Pedro J. Pérez,^b Dmitry S. Yufit^c

^a Universitetskii pr. 26 , 198504 St. Petersburg, Russia. Fax: +7 812 4286939; Tel: +7 812 4284021; E-mail: alexander.khlebnikov@pobox.spbu.ru

^b Laboratorio de Catálisis Homogénea, Departamento de Química y Ciencias de los Materiales, Unidad Asociada al CSIC, Centro de Investigación en Química Sostenible (CIQSO), Universidad de Huelva, Campus de El Carmen s/n, 21007 Huelva, Spain. Fax: +34-959219942; Tel: +34 959 219956; E-mail: perez@dqcm.uhu.es

^c Department of Chemistry, University of Durham, Durham, South Rd., DH1 3L (UK) . Fax: +44 191-334-2051; Tel: +44 191-334-2004; E-mail: d.s.yufit@durham.ac.uk

Pages 1-6: X-Ray crystal structure of *exo*-2a.
Pages 7: 2D-¹H-NOESY spectra of compound 4.
Pages 8-38: Computational details.



X-Ray crystal structure of compound *exo*-2a.

Table 1 Crystal data and structure refinement for compound *exo-2a*.

Identification code	dk48
Empirical formula	C ₂₅ H ₂₂ NO ₅ Br
Formula weight	496.35
Temperature	120(2)
Crystal system	Triclinic
Space group	P-1
a/Å, b/Å, c/Å	8.1931(2), 11.5561(3), 13.5965(4)
α/°, β/°, γ/°	65.46(1), 89.46(1), 70.36(1)
Volume/Å ³	1090.13(5)
Z	2
ρ _{calc} /mg/mm ³	1.512
m/mm ⁻¹	1.923
F(000)	508
Crystal size	0.3 × 0.2 × 0.15
Theta range for data collection	1.67 to 30.50°
Index ranges	-11 ≤ h ≤ 11, -16 ≤ k ≤ 16, -19 ≤ l ≤ 19
Reflections collected	12682
Independent reflections	6586[R(int) = 0.0155]
Data/restraints/parameters	6586/0/377
Goodness-of-fit on F ²	1.097
Final R indexes [I > 2σ (I)]	R ₁ = 0.0283, wR ₂ = 0.0671
Final R indexes [all data]	R ₁ = 0.0358, wR ₂ = 0.0700
Largest diff. peak/hole	0.403/-0.273

Table 2 Atomic Coordinates ($\text{\AA} \times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for dk48. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Br1	-3900.9(2)	12505.5(16)	-5246.6(12)	33.02(5)
O1	1611.9(12)	5844(9)	174.6(7)	15.73(17)
O2	1631.5(11)	7367.4(9)	905.9(7)	15.15(16)
O3	1463.2(15)	2312.4(10)	5041.3(8)	27.2(2)
O4	-3279.4(12)	7080.6(9)	1122(8)	18.27(18)
O5	-2562.5(13)	8752.9(10)	1224.1(8)	23.2(2)
N1	-597.8(13)	8788.4(11)	-498.9(8)	14.77(19)
C1	2515.1(15)	6476.1(12)	-605.4(10)	14.9(2)
C2	3551.5(16)	5730.9(13)	-1112.1(10)	17.4(2)
C3	4510.3(17)	6330(14)	-1878.8(11)	19.1(2)
C4	4459.7(17)	7640.1(14)	-2119.7(11)	20.1(2)
C5	3424.5(16)	8367.1(13)	-1598(11)	18(2)
C6	2426.9(15)	7793.2(13)	-844.1(10)	15.4(2)
C7	1297.3(16)	8429.4(12)	-186.8(10)	14.7(2)
C8	-1046.7(15)	7601.1(12)	153.7(9)	13.9(2)
C9	769.7(15)	6535.5(12)	824(10)	14.2(2)
C10	836.8(15)	5442.5(12)	1934.9(10)	15.1(2)
C11	622.2(17)	4257.7(13)	2038.1(11)	18.7(2)
C12	802.2(18)	3192.9(14)	3061.8(11)	21.5(3)
C13	1203.9(17)	3314.3(14)	3998.1(10)	20(2)
C14	1366.6(19)	4517.4(15)	3901.8(11)	22.3(3)
C15	1189.2(17)	5568.3(14)	2880.2(11)	19.1(2)
C16	1700(3)	983(16)	5155.3(14)	35.1(4)
C17	-2380.3(15)	7904.3(12)	891.8(10)	15.5(2)
C18	-4488.3(17)	7122.7(15)	1919.1(12)	22(3)
C19	-3526(2)	6251.5(18)	3067.8(13)	32.6(3)
C20	-1402.9(16)	9657.2(12)	-1578.8(10)	14.9(2)
C21	-2905.1(17)	9600.7(13)	-2011.9(11)	18.6(2)
C22	-3671.3(18)	10465.2(14)	-3094(11)	21.3(3)
C23	-2944.1(18)	11387.9(14)	-3748.9(10)	20.9(2)
C24	-1497.4(18)	11497.1(13)	-3324.7(11)	19.7(2)
C25	-739.2(17)	10645.4(13)	-2244.7(10)	17.7(2)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for dk48. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*U_{11} + \dots + 2hka^*b^*U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br1	42.79(10)	28.9(9)	17.89(7)	-1.57(6)	-5.24(6)	-12.8(7)
O1	19.2(4)	14.5(4)	16.6(4)	-8.4(3)	6.3(3)	-7.8(3)
O2	16.5(4)	16(4)	15.4(4)	-7.4(3)	1.2(3)	-8.2(3)
O3	36.1(6)	22(5)	17.1(4)	-2.9(4)	5.5(4)	-10.5(4)
O4	16.9(4)	19.7(4)	24.7(5)	-12.7(4)	7.7(3)	-10.6(4)
O5	26.2(5)	23.3(5)	32(5)	-18.9(4)	12.3(4)	-14.4(4)
N1	13.5(4)	13.9(5)	16.2(5)	-5(4)	1.6(4)	-6.2(4)
C1	14.3(5)	16.1(5)	14(5)	-6(4)	0.9(4)	-5.8(4)
C2	17.7(6)	17.7(6)	17.8(5)	-8.8(5)	2.7(4)	-6.1(5)
C3	18.4(6)	21.4(6)	18.5(6)	-10.1(5)	4.6(5)	-6.5(5)
C4	18.4(6)	22.7(6)	20.8(6)	-9.4(5)	6.6(5)	-9.7(5)
C5	17.4(6)	17.3(6)	21(6)	-8.5(5)	3.8(5)	-8.2(5)
C6	13.5(5)	16.4(6)	17.2(5)	-7.9(5)	1.7(4)	-5.8(4)
C7	15.2(5)	14.6(5)	16.4(5)	-7.6(5)	2(4)	-6.7(4)
C8	14.8(5)	13(5)	15.2(5)	-6.3(4)	2(4)	-6.6(4)
C9	14.7(5)	15.1(5)	14.9(5)	-8(4)	2.2(4)	-5.9(4)
C10	12.7(5)	15.3(5)	15.6(5)	-6.3(4)	2.4(4)	-3.8(4)
C11	22.7(6)	18.7(6)	17.2(6)	-8.4(5)	4.2(5)	-9.9(5)
C12	26.1(7)	18.4(6)	21(6)	-7.5(5)	5.9(5)	-10.6(5)
C13	19.4(6)	19.4(6)	16.5(6)	-4.3(5)	4.6(5)	-5.9(5)
C14	26.6(7)	23.5(7)	16.3(6)	-8.7(5)	2.3(5)	-8.8(5)
C15	22.5(6)	18.4(6)	18(6)	-8.9(5)	2.4(5)	-8.2(5)
C16	50.5(10)	19.5(7)	25.8(7)	-3.5(6)	12.1(7)	-9.8(7)
C17	13.8(5)	14.7(5)	17.4(5)	-6.2(5)	1.1(4)	-5.7(4)
C18	17.1(6)	24.6(7)	29(7)	-14(6)	10.1(5)	-10.6(5)
C19	28.3(8)	33.7(9)	25.9(7)	-7.2(7)	10.6(6)	-7.3(7)
C20	15.4(5)	12.8(5)	15.7(5)	-6.6(4)	2.2(4)	-3.7(4)
C21	17.5(6)	17.8(6)	19.8(6)	-6.5(5)	2.1(5)	-8(5)
C22	19.9(6)	20.5(6)	21.7(6)	-7.6(5)	-1.7(5)	-7.1(5)
C23	24.8(6)	18.1(6)	15.6(5)	-5.6(5)	0.7(5)	-5.1(5)
C24	23(6)	16.3(6)	18.9(6)	-6.6(5)	5(5)	-7.6(5)
C25	18.6(6)	16.1(6)	19.5(6)	-7.9(5)	3.4(5)	-7.3(5)

Table 4 Bond Lengths for dk48.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C23	1.8960(13)	C5	C6	1.3937(17)
O1	C1	1.3824(14)	C6	C7	1.5061(16)
O1	C9	1.4484(14)	C8	C17	1.5290(16)
O2	C9	1.4078(14)	C8	C9	1.5567(17)
O2	C7	1.4338(15)	C9	C10	1.5001(16)
O3	C13	1.3689(15)	C10	C11	1.3882(17)
O3	C16	1.4227(19)	C10	C15	1.3952(17)
O4	C17	1.3290(14)	C11	C12	1.3902(18)
O4	C18	1.4659(15)	C12	C13	1.3915(18)
O5	C17	1.2068(15)	C13	C14	1.3931(19)
N1	C20	1.3957(15)	C14	C15	1.3818(18)
N1	C8	1.4584(15)	C18	C19	1.503(2)
N1	C7	1.4820(15)	C20	C21	1.4021(17)
C1	C2	1.3883(17)	C20	C25	1.4031(17)
C1	C6	1.3940(17)	C21	C22	1.3899(18)
C2	C3	1.3907(17)	C22	C23	1.3832(19)
C3	C4	1.3955(19)	C23	C24	1.3883(19)
C4	C5	1.3903(18)	C24	C25	1.3844(18)

Table 5 Bond Angles for dk48.

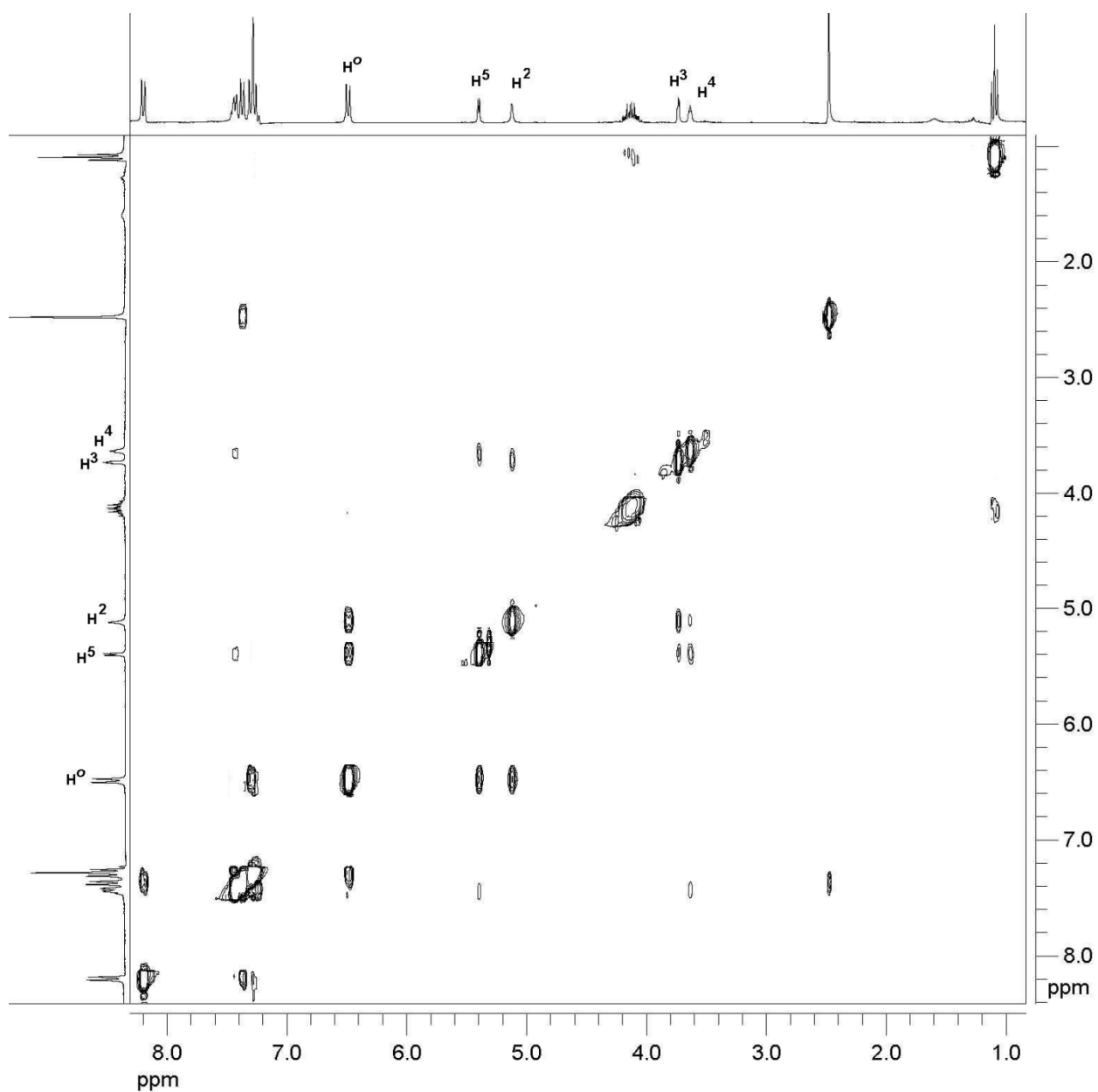
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	O1	C9	116.87(9)	O1	C9	C8	107.11(9)
C9	O2	C7	103.68(8)	C10	C9	C8	118.95(10)
C13	O3	C16	116.80(12)	C11	C10	C15	118.86(12)
C17	O4	C18	117.34(10)	C11	C10	C9	120.15(11)
C20	N1	C8	121.11(10)	C15	C10	C9	120.92(11)
C20	N1	C7	120.25(10)	C10	C11	C12	120.99(12)
C8	N1	C7	108.15(9)	C11	C12	C13	119.60(12)
O1	C1	C2	117.33(11)	O3	C13	C12	124.27(12)
O1	C1	C6	121.03(10)	O3	C13	C14	116.01(12)
C2	C1	C6	121.62(11)	C12	C13	C14	119.71(12)
C1	C2	C3	118.47(12)	C15	C14	C13	120.19(12)
C2	C3	C4	120.87(12)	C14	C15	C10	120.59(12)
C5	C4	C3	119.84(12)	O5	C17	O4	125.52(11)
C4	C5	C6	120.03(12)	O5	C17	C8	124.71(11)
C1	C6	C5	119.15(11)	O4	C17	C8	109.76(10)
C1	C6	C7	114.55(10)	O4	C18	C19	110.81(11)
C5	C6	C7	126.21(11)	N1	C20	C21	121.59(11)
O2	C7	N1	101.86(9)	N1	C20	C25	119.76(11)
O2	C7	C6	106.38(10)	C21	C20	C25	118.62(11)
N1	C7	C6	112.80(9)	C22	C21	C20	120.54(12)
N1	C8	C17	111.49(9)	C23	C22	C21	119.70(12)
N1	C8	C9	101.51(9)	C22	C23	C24	120.66(12)
C17	C8	C9	111.99(9)	C22	C23	Br1	120.14(10)
O2	C9	O1	111.30(9)	C24	C23	Br1	119.19(10)
O2	C9	C10	110.35(9)	C25	C24	C23	119.76(12)
O1	C9	C10	106.66(9)	C24	C25	C20	120.59(12)
O2	C9	C8	102.43(9)				

Table 8 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for dk48.

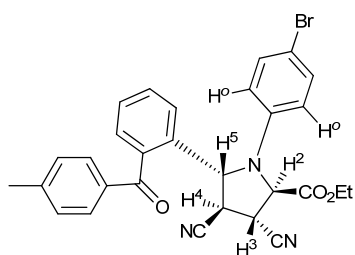
Atom	x	y	z	U(eq)
H7	1520(2)	9171(16)	-177(12)	13(3)
H5	3380(2)	9242(17)	-1741(13)	20(4)
H2	3590(2)	4804(17)	-919(13)	19(4)
H8	-1470(2)	7233(16)	-283(13)	15(4)
H182	-5100(2)	8071(17)	1761(13)	16(4)
H15	1330(2)	6340(2)	2816(15)	34(5)
H21	-3420(2)	8981(17)	-1566(14)	22(4)
H4	5160(2)	8002(17)	-2644(14)	22(4)
H24	-1030(2)	12161(18)	-3791(15)	28(4)
H11	360(2)	4159(18)	1415(15)	29(5)
H3	5240(2)	5805(18)	-2196(14)	25(4)
H25	230(2)	10756(17)	-1955(13)	21(4)
H22	-4740(3)	10428(19)	-3358(15)	32(5)
H181	-5320(3)	6816(19)	1732(15)	33(5)
H12	680(2)	2410(2)	3106(15)	34(5)
H14	1640(2)	4582(19)	4572(16)	33(5)
H162	1970(3)	380(2)	5920(18)	42(5)
H191	-2820(3)	5380(2)	3139(18)	48(6)

Crystal structure determination of [dk48]

Crystal Data. $\text{C}_{25} \text{H}_{22} \text{Br N O}_5$, $M = 496.35$, Triclinic, $a = 8.1931(2)$, $b = 11.5561(3)$, $c = 13.5965(4)$, $\alpha = 65.4650(10)$, $\beta = 89.4570(10)$, $\gamma = 70.3560(10)$, $U = 1090.13(5) \text{\AA}^3$, $T = 120(2)$, space group P-1 (no. 2), $Z = 2$, $\mu(\text{Mo-K}\alpha) = 1.923$, 12682 reflections measured, 6586 unique ($R_{\text{int}} = 0.0155$) which were used in all calculations. The final $wR(F_2)$ was 0.0700 (all data).



2D ^1H NOESY spectrum of compound 4.



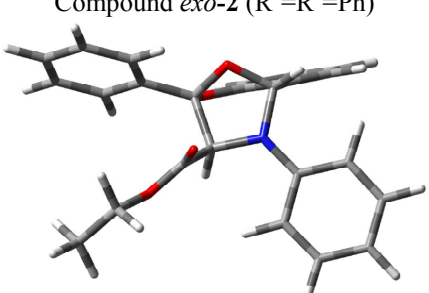
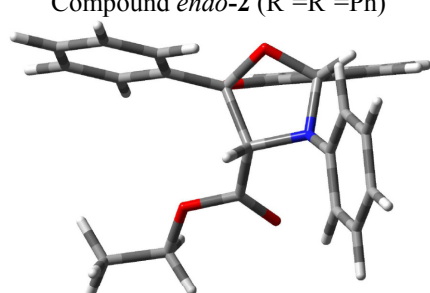
Computational Details

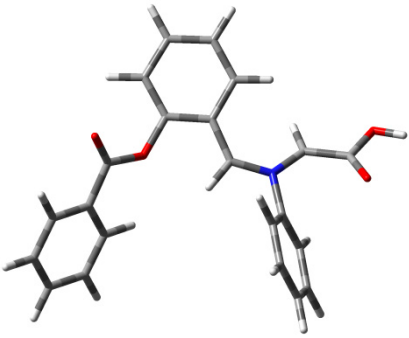
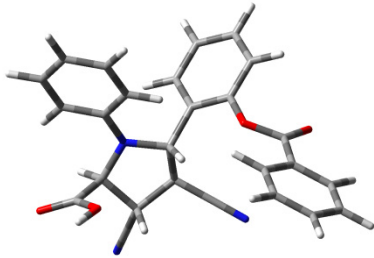
All calculations were performed with the B3LYP density functional method¹ by using the Gaussian suite of quantum chemical programs. Geometry optimizations of intermediates, transition states, reactants, and products in the gas phase were performed at the B3LYP/6-31G(d) level using Gaussian 03.² Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate. Intrinsic reaction coordinates (IRC) were calculated to authenticate all transition states.

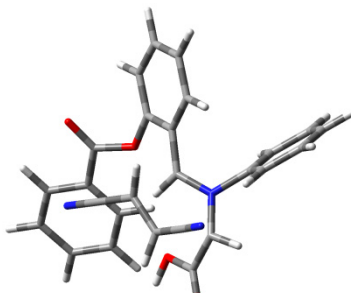
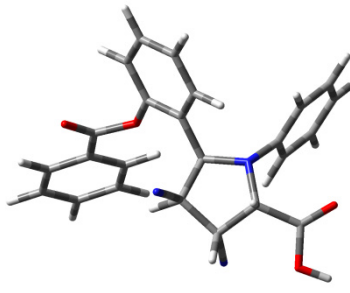
¹ (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *Phys. Rev. A* **1998**, *38*, 3098. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1998**, *37*, 785.

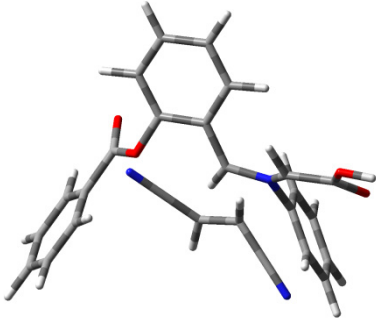
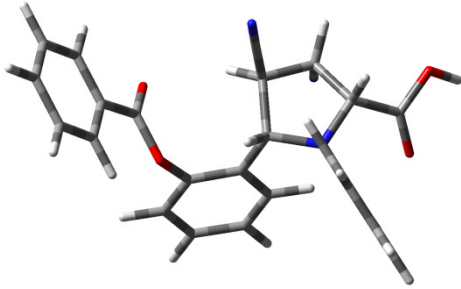
² Frisch, M.J.; Trucks, G.W. Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Montgomery, J.A. Jr.; Vreven, T.; Kudin, K.N.; Burant, J.C.; Millam, J.M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin, A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Ayala, P.Y.; Morokuma, K.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Zakrzewski, V.G.; Dapprich, S.; Daniels, A.D.; Strain, M.C.; Farkas, O.; Malick, D.K.; Rabuck, A.D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J.V.; Cui, Q.; Baboul, A.G.; Clifford, S.; Cioslowski, J.; Stefanov, B.B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R.L.; Fox, D.J.; Keith, T.; Al-Laham, M. A.; Peng, C.Y.; Nanayakkara, A.; Challacombe, M.; Gill, P.M.W.; Johnson, B.; Chen, W.; Wong, M.W.; Gonzalez, C.; Pople, J.A. Gaussian 03, Revision B.05, Gaussian, Inc., Pittsburgh PA, **2003**.

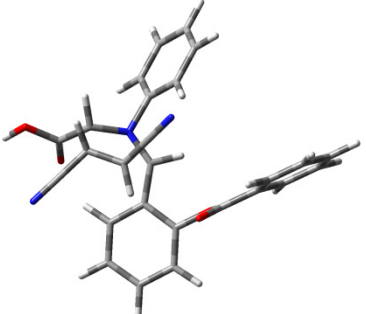
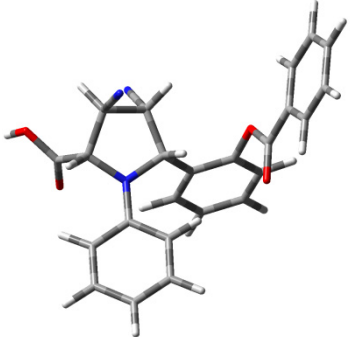
Table. B3LYP/6-31G(d) Absolute Energies (au), Cartesian Coordinates of stationary points of compounds and transition states of isomerizations and cycloadditions

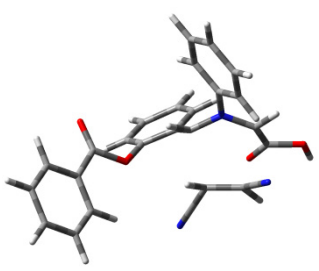
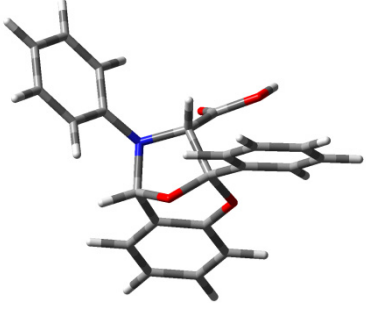
Compound <i>exo-2</i> ($R^1=R^2=Ph$)				Compound <i>endo-2</i> ($R^1=R^2=Ph$)			
							
E = -1282.84251599, H (0K) = -1282.440449, H (298K) = -1282.415796, G (298K) = -1282.495992 au.				E = -1282.84019889, H (0K) = -1282.438337, H (298K) = -1282.413660, G (298K) = -1282.494297 au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	-2.9365380	-3.6987180	-1.4001170	C	0.2765880	4.7467760	-0.4736550
C	-3.7621180	-3.1889040	-0.3964480	C	-1.0836660	4.6225270	-0.7685080
C	-3.2613540	-2.2301740	0.4883930	C	-1.6252690	3.3584590	-1.0056460
C	-1.9531860	-1.7701700	0.3625840	C	-0.8219850	2.2218500	-0.9392110
C	-1.1336640	-2.2985160	-0.6466820	C	0.5376620	2.3635960	-0.6351860
C	-1.6150200	-3.2656850	-1.5257960	C	1.0962280	3.6201210	-0.4103930
C	-1.2801680	-0.7415920	1.2445720	C	-1.3064260	0.8155480	-1.2090460
O	0.0599340	-1.1971670	1.4502970	O	-0.2111520	0.1216480	-1.8573820
C	0.6764940	-0.9701500	0.2083680	C	0.7225650	-0.0003740	-0.8111180
O	0.1729080	-1.8900190	-0.7851050	O	1.3627640	1.2626530	-0.5643530
N	-1.0715060	0.5396370	0.5656750	N	-1.5295830	0.0750960	0.0196060
C	0.1744470	0.4736680	-0.1722170	C	-0.2003690	-0.3906080	0.4282770
C	1.1556890	1.5695880	0.2645620	C	0.2900290	0.1897140	1.7550320
O	1.2455810	2.0221240	1.3812950	O	-0.2726820	1.0314190	2.4146880
O	1.9226730	1.9402000	-0.7798930	O	1.4444400	-0.4116450	2.1078570
H	-3.3182020	-4.4466170	-2.0897720	H	0.7062090	5.7282840	-0.2927510
H	-4.7859070	-3.5372150	-0.2988400	H	-1.7157140	5.5040370	-0.8198040
H	-3.8925470	-1.8397800	1.2830000	H	-2.6806820	3.2511380	-1.2462080
H	-0.9547580	-3.6660360	-2.2886110	H	2.1558290	3.6980180	-0.1880710
H	-1.7538040	-0.6197640	2.2209620	H	-2.1753170	0.7974940	-1.8649640
H	0.0457710	0.5242040	-1.2589860	H	-0.1944380	-1.4805940	0.5249180
C	-2.0728960	1.4672270	0.2955050	C	-2.6048370	-0.8524870	0.1254720
C	-1.8497800	2.5260010	-0.6080110	C	-3.0338460	-1.2028000	1.4152050
C	-3.3255420	1.3948770	0.9379070	C	-3.2451520	-1.4258050	-0.9837440
C	-2.8434040	3.4723570	-0.8487560	C	-4.0737700	-2.1134080	1.5904180
H	-0.8976790	2.6179760	-1.1198710	H	-2.5576090	-0.7284430	2.2680500
C	-4.3075590	2.3489240	0.6855570	C	-4.3034790	-2.3172230	-0.7993730
H	-3.5342160	0.5971810	1.6420710	H	-2.9065110	-1.2013820	-1.9906930
C	-4.0806520	3.3957710	-0.2091540	C	-4.7204010	-2.6700440	0.4844710
H	-2.6410960	4.2788200	-1.5491330	H	-4.3938840	-2.3719050	2.5964630
H	-5.2632890	2.2669510	1.1971190	H	-4.7906040	-2.7510930	-1.6688980
H	-4.8516510	4.1352960	-0.4033490	H	-5.5404360	-3.3692060	0.6217260
C	2.1723200	-1.1666340	0.3031380	C	1.7873190	-1.0130480	-1.1644710
C	2.8329640	-0.8944480	1.5067340	C	3.1230460	-0.8202080	-0.7993940
C	2.9060590	-1.5833040	-0.8132660	C	1.4203990	-2.1768160	-1.8510180
C	4.2176550	-1.0449840	1.5911210	C	4.0811120	-1.7831880	-1.1190960
H	2.2611610	-0.5674540	2.3674720	H	3.4072710	0.0841390	-0.2750700
C	4.2902560	-1.7286830	-0.7240440	C	2.3803620	-3.1364830	-2.1685980
H	2.3916900	-1.8043760	-1.7417570	H	0.3858780	-2.3195040	-2.1467170
C	4.9491590	-1.4608240	0.4774730	C	3.7139800	-2.9428030	-1.8028020
H	4.7228150	-0.8391770	2.5308420	H	5.1180200	-1.6230230	-0.8356830
H	4.8529180	-2.0578330	-1.5935140	H	2.0864250	-4.0333450	-2.7072490
H	6.0274070	-1.5787300	0.5459930	H	4.4623830	-3.6903340	-2.0521100
C	2.9673260	2.9014170	-0.4891730	C	2.0454650	0.0426210	3.3441230
C	3.7399770	3.1351550	-1.7730120	C	3.2758680	-0.8089090	3.5924410

H	3.6001220	2.4949490	0.3055630	H	1.3084060	-0.0513440	4.1476970
H	2.5020860	3.8173790	-0.1114040	H	2.2911890	1.1046080	3.2420380
H	4.5438010	3.8580070	-1.5957190	H	3.7687230	-0.4879720	4.5166660
H	4.1868660	2.2028270	-2.1323010	H	3.0064480	-1.8650490	3.6935490
H	3.0874950	3.5316220	-2.5576660	H	3.9899860	-0.7148450	2.7683250
Ylide S-3' (X=Y=H)				(2<i>RS</i>,3<i>RS</i>,4<i>RS</i>,5<i>RS</i>)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid			
							
E = -1204.19794783, H (0K) = -1203.855921, H (298K) = -1203.83236, G (298K) = -1203.912177 au. Imaginary frequency = 0.				E = -1467.33383803, H (0K) = -1466.935185, H (298K) = -1466.906242, G (298K) = -1466.998033 au. Imaginary frequency = 0.			
C	0.3790010	1.9039310	0.0010860	C	-0.1596920	1.2133830	-1.2239890
C	-1.0117650	2.1675210	-0.0992140	C	1.1468930	1.6819370	-1.0306880
C	0.8023040	0.5229350	0.0250370	C	-0.6295470	-0.0904940	-0.5962910
O	-3.3059990	1.5591400	1.3264030	O	3.7243280	0.8629310	-1.5585750
C	-2.9705880	0.8558100	0.4015610	C	3.2354230	0.6125590	-0.4834920
O	-1.8377170	1.0714490	-0.3499780	O	1.9480300	0.9762480	-0.1336950
N	2.0391800	0.0274200	-0.1330670	N	-2.0234810	-0.0605510	-0.1433060
C	3.1089060	0.6940840	-0.6648470	C	-2.7132420	-1.3386920	-0.3123180
C	4.4721740	0.3385520	-0.3998850	C	-3.1611760	-2.0018720	0.9981260
O	4.9135760	-0.5397910	0.3326420	O	-4.2710630	-2.4302030	1.2018660
O	5.3207190	1.1670610	-1.1004280	O	-2.1450000	-2.0837390	1.8877810
H	0.0403230	-0.2287010	0.1654020	H	0.0569910	-0.3733770	0.2119820
H	2.8897430	1.5811150	-1.2373220	H	-3.6185920	-1.2378160	-0.9206220
H	6.2119350	0.8700260	-0.8438630	H	-2.5068050	-2.5077890	2.6888410
C	-1.5313040	3.4545090	-0.0388580	C	1.5950160	2.8571790	-1.6352420
C	-0.6700750	4.5358590	0.1437350	C	0.7300410	3.5747340	-2.4576440
H	-1.0729560	5.5432960	0.1867700	H	1.0786350	4.4873790	-2.9322690
C	0.7042070	4.3148870	0.2609440	C	-0.5765820	3.1275910	-2.6649750
C	1.2218950	3.0283890	0.1754520	C	-1.0126640	1.9585330	-2.0477670
H	1.3805450	5.1516930	0.4099470	H	-1.2547490	3.6912060	-3.2988200
H	2.2902390	2.8819640	0.2742150	H	-2.0354780	1.6184760	-2.1826040
H	-2.6001240	3.6039120	-0.1296420	H	2.6098690	3.1942770	-1.4659430
C	2.1778660	-1.3851780	0.2027130	C	-2.4749800	0.8600930	0.8255320
C	1.8075460	-1.8233210	1.4718670	C	-1.5827240	1.6697630	1.5489140
C	2.6199480	-2.2790830	-0.7716740	C	-3.8543190	0.9883140	1.0757420
C	1.8875330	-3.1839920	1.7720570	C	-2.0632800	2.5842830	2.4853660
H	1.4843980	-1.1033890	2.2169170	H	-0.5141590	1.5902620	1.3880790
C	2.6910370	-3.6347720	-0.4642280	C	-4.3191450	1.8957910	2.0254360
H	2.9002670	-1.9069020	-1.7514840	H	-4.5689470	0.3838790	0.5264760
C	2.3273050	-4.0896740	0.8067170	C	-3.4303720	2.7045370	2.7348520
H	1.6121000	-3.5312040	2.7636730	H	-1.3534270	3.2014710	3.0299050
H	3.0302390	-4.3384550	-1.2189770	H	-5.3887780	1.9733880	2.2009950
H	2.3896270	-5.1482630	1.0428010	H	-3.7970300	3.4155520	3.4692220
C	-3.7083260	-0.3473870	-0.0674270	C	3.9144880	-0.1098940	0.6227230
C	-3.2959200	-1.1090700	-1.1707350	C	3.3516790	-0.2502600	1.8996380
C	-4.8636930	-0.7117990	0.6393470	C	5.1782750	-0.6554230	0.3538090
C	-4.0353600	-2.2251340	-1.5580850	C	4.0502500	-0.9307120	2.8950130
H	-2.4048540	-0.8235930	-1.7181120	H	2.3778280	0.1767480	2.1104830
C	-5.5979170	-1.8279170	0.2487500	C	5.8693830	-1.3387910	1.3501450
H	-5.1669030	-0.1083310	1.4884990	H	5.5960410	-0.5367340	-0.6402440
C	-5.1845190	-2.5857660	-0.8503890				
H	-3.7150080	-2.8136880	-2.4131610				

H	-6.4918720	-2.1077580	0.7988990	C	5.3067910	-1.4764930	2.6219190
H	-5.7581340	-3.4568450	-1.1557400	H	3.6141960	-1.0353570	3.8845790
				H	6.8455290	-1.7646850	1.1364450
				H	5.8473580	-2.0090100	3.3998850
				C	-1.6687210	-2.2505310	-1.0299370
				C	-0.6646100	-1.2386540	-1.6454310
				C	0.6484790	-1.8251660	-1.9098810
				N	1.6911020	-2.2988390	-2.0976420
				C	-2.2653320	-3.1572290	-2.0099660
				N	-2.7434430	-3.8641600	-2.7962250
				H	-1.0706620	-0.8451350	-2.5833840
				H	-1.1394400	-2.8467230	-0.2793650
<p>TS Ylide S-3' (X=Y=H) + fumaronitrile → (2<i>RS</i>,3<i>RS</i>,4<i>SR</i>,5<i>RS</i>)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p>  <p>E = -1467.26362661, H (0K) = -1466.869515, H (298K) = -1466.839987, G (298K) = -1466.931888 au. Imaginary frequency = 1.</p>				<p>(2<i>RS</i>,3<i>SR</i>,4<i>SR</i>,5<i>RS</i>)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p>  <p>E = -1467.32043780, H (0K) = -1466.922538, H (298K) = -1466.893600, G (298K) = -1466.986855 au. Imaginary frequency = 0.</p>			
C	0.5582350	1.4945720	0.3355520	C	-0.0859600	1.8043710	-0.0638130
C	-0.7033490	2.1243950	0.2236910	C	1.2355190	1.9873450	0.3663640
C	0.6227790	0.0501260	0.1115480	C	-0.5810110	0.4224490	-0.4527330
O	-3.2906260	2.1007980	1.2332370	O	3.7805520	1.7021080	-0.6741930
C	-2.9973990	1.3700810	0.3184200	C	3.2908870	0.7946590	-0.0420450
O	-1.7402460	1.3391940	-0.2596880	O	2.0223820	0.8378920	0.4908970
N	1.6403210	-0.6302700	-0.4685620	N	-2.0326060	0.2204930	-0.2442190
C	1.6816310	-2.0164960	-0.4539060	C	-2.6039930	-0.4866490	-1.4043810
C	0.5662360	-2.9156330	-0.7667630	C	-3.7657910	-1.4385050	-1.1438840
O	0.7146420	-4.1127750	-0.9295590	O	-4.5896130	-1.3401330	-0.2700230
O	-0.6621120	-2.3276540	-0.8222770	O	-3.8250880	-2.3768430	-2.1212660
H	-0.3218610	-0.4649350	0.0912700	H	-0.0128810	-0.3146730	0.1273220
H	2.6335880	-2.4272340	-0.7620910	H	-3.0400300	0.2558860	-2.0953310
H	-1.3004620	-3.0488030	-0.9769750	H	-4.6206850	-2.9137480	-1.9413940
C	-0.8694530	3.4817300	0.4934450	C	1.7197370	3.2413550	0.7343320
C	0.2277980	4.2359570	0.9032350	C	0.8736540	4.3458120	0.6551120
H	0.0981410	5.2926530	1.1183240	H	1.2475680	5.3261530	0.9361240
C	1.4828040	3.6376910	1.0425620	C	-0.4434080	4.1917230	0.2199020
C	1.6437250	2.2863250	0.7622890	C	-0.9154430	2.9287830	-0.1307350
H	2.3344930	4.2229670	1.3759830	H	-1.1031120	5.0521240	0.1566210
H	2.6181400	1.8292900	0.8883010	H	-1.9415500	2.7937120	-0.4554190
H	-1.8470220	3.9332530	0.3903880	H	2.7447550	3.3471590	1.0673270
C	2.8365250	0.0362310	-0.9646780	C	-2.3979900	-0.1155590	1.1128920
C	2.7003870	0.8651390	-2.0809970	C	-1.9570750	-1.2934370	1.7311000
C	4.0866260	-0.1830300	-0.3828070	C	-3.1686280	0.7941960	1.8413830
C	3.8262140	1.4934910	-2.6103280	C	-2.2907140	-1.5542790	3.0602740
H	1.7217570	1.0107900	-2.5266800	H	-1.3646120	-2.0139130	1.1732440
C	5.2075040	0.4497180	-0.9256750	C	-3.5019170	0.5313610	3.1701320
H	4.1921010	-0.8319970	0.4803330	H	-3.5052020	1.7033350	1.3540350
C	5.0814450	1.2886570	-2.0333380	C	-3.0623760	-0.6427750	3.7830910
H	3.7210350	2.1372140	-3.4787700	H	-1.9501630	-2.4737290	3.5289670
H	6.1804090	0.2820230	-0.4731770	H	-4.1043330	1.2447500	3.7259290

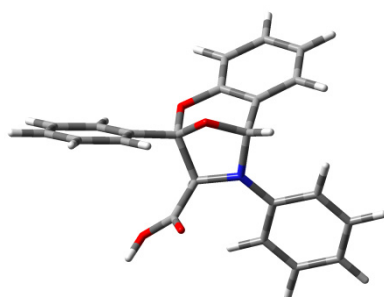
H	5.9578820	1.7772550	-2.4491390	H	-3.3205360	-0.8476290	4.8185730
C	-3.9144340	0.4079240	-0.3443660	C	3.9595900	-0.5016430	0.2473180
C	-3.5328190	-0.3706500	-1.4471290	C	3.3630180	-1.5116010	1.0164360
C	-5.2141690	0.3001160	0.1704530	C	5.2429810	-0.6960770	-0.2850090
C	-4.4500120	-1.2445410	-2.0280590	C	4.0466290	-2.7042110	1.2456430
H	-2.5257200	-0.2928610	-1.8393390	H	2.3733640	-1.3607370	1.4318530
C	-6.1243790	-0.5779400	-0.4110340	C	5.9211860	-1.8890200	-0.0528350
H	-5.4872530	0.9076650	1.0266050	H	5.6875600	0.0980790	-0.8755770
C	-5.7442070	-1.3497670	-1.5119870	C	5.3234060	-2.8944800	0.7121760
H	-4.1569120	-1.8422400	-2.8870690	H	3.5815650	-3.4861460	1.8389740
H	-7.1290730	-0.6619240	-0.0068060	H	6.9145010	-2.0366550	-0.4671320
H	-6.4556690	-2.0335080	-1.9673890	H	5.8525790	-3.8264300	0.8921830
C	1.4871710	-2.2772000	1.8128210	C	-1.3912220	-1.0853040	-2.1739930
C	0.8290460	-1.1133590	2.2356390	H	-1.6217670	-1.2378120	-3.2314710
C	-0.5686120	-1.1263990	2.5013280	C	-0.3401020	0.0454880	-1.9501320
N	-1.7193480	-1.1225130	2.6906260	H	0.6854830	-0.3067540	-2.0922180
C	2.8850810	-2.4207120	2.0813030	C	-0.5936220	1.1388120	-2.8944880
N	4.0268040	-2.5099280	2.2965260	N	-0.8223280	1.9713310	-3.6702140
H	1.3952800	-0.2958400	2.6685470	C	-0.9054230	-2.3487940	-1.6114350
H	0.9372070	-3.2098420	1.7365400	N	-0.4936300	-3.3305770	-
<p>TS Ylide S-3' (X=Y=H) + fumaronitrile → (2RS,3SR,4SR,5RS)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p> 				<p>(2RS,3RS,4RS, 5SR)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p> 			
<p>E = -1467.25808288, H (0K) = -1466.864092, H (298K) = -1466.834529, G (298K) = -1466.926753 au. Imaginary frequency = 1.</p>				<p>E = -1467.33299832, H (0K) = -1466.934529, H (298K) = -1466.905713, G (298K) = -1466.905713 au. Imaginary frequency = 0.</p>			
C	-0.0181650	1.7233060	-0.7091310	C	0.2190090	-1.0872030	1.0773130
C	-1.4151220	1.9026110	-0.6104270	C	-1.0748310	-1.2739300	1.5791680
C	0.5211170	0.3925880	-0.4472690	C	0.4808350	-0.0572450	-0.0186770
O	-3.4689340	0.6823790	-1.9733760	O	-2.6531960	-1.8129620	-0.5716800
C	-3.2284540	0.3485510	-0.8366720	C	-2.9100260	-0.8421270	0.1097800
O	-2.1585400	0.8389930	-0.1143050	O	-2.1225350	-0.4369430	1.1557280
N	1.8358680	0.0358160	-0.4882460	N	1.8851320	0.3725060	-0.0902880
C	2.7541420	0.7747820	0.2224940	C	2.5079850	0.0381980	-1.3590900
C	4.2094190	0.5926510	0.0849560	C	3.9382390	-0.4871150	-1.2094860
O	4.8126280	-0.2246700	-0.5787580	O	4.4894560	-0.7957270	-0.1812480
O	4.8388590	1.5127030	0.8691700	O	4.5196030	-0.5789740	-2.4284150
H	-0.1550190	-0.4313610	-0.6327810	H	-0.1673980	0.8029490	0.1736680
H	2.4555230	1.7949880	0.3991480	H	2.5551700	0.9012200	-2.0426540
H	5.7923200	1.3268100	0.7843590	H	5.4065240	-0.9617550	-2.2883550
C	-1.2544260	4.1728670	-1.3864880	C	-1.3533330	-2.2027260	2.5760900
C	-2.0287620	3.1072940	-0.9375920	C	1.2455740	-1.8638330	1.6260570
H	-1.7303220	5.1162790	-1.6362270	C	0.9817460	-2.8058500	2.6202580
C	0.7368700	2.8200340	-1.1776340	H	1.7953640	-3.4008900	3.0244270
C	0.1293870	4.0229430	-1.5147050	C	-0.3182930	-2.9794460	3.0951350
H	0.7364870	4.8444210	-1.8832280	H	-0.5290770	-3.7090690	3.8717140
H	1.8063900	2.7152050	-1.3231440	H	-2.3716250	-2.2992050	2.9394900
H	-3.1036000	3.2010420	-0.8366040	H	2.2585320	-1.7111990	1.2695080
C	2.0956520	-1.3042970	-0.9893050				

C	2.7173310	-2.2918150	-0.2233920	C	2.2278140	1.6523830	0.4733010
C	1.6411080	-1.5853160	-2.2816490	C	1.6179920	2.8308870	0.0177370
C	2.8739970	-3.5677340	-0.7625740	C	3.1987980	1.7194790	1.4773040
H	3.0806360	-2.0820230	0.7736590	C	1.9709570	4.0609500	0.5727820
C	1.8038700	-2.8653310	-2.8099410	H	0.8710220	2.7853830	-0.7718220
H	1.1803620	-0.7994310	-2.8720520	C	3.5542170	2.9540810	2.0240320
C	2.4189910	-3.8601450	-2.0498370	H	3.6704160	0.8009950	1.8080580
H	3.3553350	-4.3362950	-0.1651770	C	2.9399210	4.1247810	1.5769040
H	1.4543390	-3.0780980	-3.8159580	H	1.4925960	4.9692500	0.2163230
H	2.5470630	-4.8582120	-2.4590550	H	4.3093730	2.9986400	2.8041880
C	-4.0017650	-0.6391020	-0.0425770	H	3.2150910	5.0839360	2.0071780
C	-3.8069080	-0.8109080	1.3361880	C	-4.0786230	0.0526100	-0.0870890
C	-4.9706570	-1.3984020	-0.7148970	C	-4.3548440	1.1291050	0.7687000
C	-4.5756880	-1.7432870	2.0306250	C	-4.9252180	-0.2133950	-1.1731270
H	-3.0741360	-0.2034060	1.8560730	C	-5.4696180	1.9312440	0.5340370
C	-5.7294180	-2.3331130	-0.0165510	H	-3.6991830	1.3292510	1.6085360
H	-5.1122390	-1.2411690	-1.7792030	C	-6.0372040	0.5913590	-1.4026450
C	-5.5319360	-2.5065680	1.3564010	H	-4.6938790	-1.0511880	-1.8223620
H	-4.4309720	-1.8715110	3.0995440	C	-6.3099990	1.6642540	-0.5496310
H	-6.4759990	-2.9244510	-0.5390790	H	-5.6833550	2.7651540	1.1965930
H	-6.1272100	-3.2341280	1.9017130	H	-6.6902190	0.3850130	-2.2457500
C	2.0031830	0.4624190	2.2875500	H	-7.1779700	2.2929070	-0.7296490
H	2.3269160	1.4408670	2.6311770	C	1.5665030	-1.0202180	-2.0128800
C	0.6255610	0.2514410	2.0861250	C	0.1695100	-0.6050600	-1.4574510
H	0.2350910	-0.7604810	2.0627200	C	-0.3927200	0.4571270	-2.2979560
C	-0.3016660	1.2833710	2.3765040	N	-0.8139020	1.3217370	-2.9492280
N	-1.0668400	2.1318010	2.6154870	C	1.9002640	-2.4103930	-1.6816550
C	2.8366430	-0.6081540	2.7427220	N	2.1764310	-3.5171870	-1.4686710
N	3.5197030	-1.4731030	3.1205780	H	1.6053450	-0.9305860	-3.1020920
				H	-0.5349120	-1.4408540	-1.4282310
<p>TS Ylide S-3' (X=Y=H) + fumaronitrile → (2<i>RS</i>,3<i>RS</i>,4<i>RS</i>, 5<i>SR</i>)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p>  <p>E = -1467.25106564, H (0K) = -1466.856875, H (298K) = -1466.827448, G (298K) = -1466.918738 au. Imaginary frequency = 1.</p>				<p>(2<i>RS</i>,3<i>SR</i>,4<i>SR</i>, 5<i>SR</i>)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p>  <p>E = -1467.33804816, H (0K) = -1466.939270, H (298K) = -1466.910530, G (298K) = -1467.001087 au. Imaginary frequency = 0.</p>			
C	-0.7170410	-1.4036300	-0.9619900	C	-0.2813870	0.0353660	1.5181300
C	0.5167780	-2.0688940	-1.1853280	C	1.0151300	0.1217690	2.0362350
C	-0.6251740	0.0091550	-0.6226230	C	-0.5066720	-0.3345620	0.0599790
O	2.0654980	-2.1182230	1.0123750	O	2.2216020	1.8778660	0.3607760
C	2.4369950	-1.4517710	0.0742000	C	2.6952610	0.7679610	0.4696180
O	1.7076150	-1.3439830	-1.0959030	O	2.1176850	-0.2186710	1.2322530
N	-1.5293840	0.9612850	-0.3256930	N	-1.8246240	0.0404730	-0.4589150
C	-2.7081460	0.8349580	0.4301950	C	-2.4654950	-1.0290940	-1.1949670
C	-3.9647110	0.3416480	-0.1592450	C	-3.6544770	-1.6507770	-0.4375190
O	-4.1393430	-0.1278900	-1.2708340	O	-4.1832470	-1.1819820	0.5399730
O	-4.9797290	0.5232020	0.7233850	O	-4.0788720	-2.7806090	-1.0514750
H	0.3248920	0.4454950	-0.9071200	H	0.2758600	0.1347240	-0.5509960
H	-2.8984280	1.7622370	0.9639110	H	-2.8703420	-0.6625170	-2.1466910
H	-5.7734010	0.1374380	0.3090840				

C	-2.0958020	-0.3667480	2.0611760	H	-4.8365870	-3.1142830	-0.5339620
C	-1.8895500	-2.1650500	-1.1374760	C	1.2556810	0.4445130	3.3668520
C	-0.7180460	-0.6561300	1.9568580	C	-1.3520370	0.2735240	2.3871700
H	-2.7507020	-4.0660880	-1.6112280	C	-1.1263820	0.5979990	3.7245780
C	-0.5969170	-4.1386470	-1.6864930	H	-1.9714950	0.7790450	4.3820530
H	-0.5505210	-5.1892360	-1.9574110	C	0.1763850	0.6880900	4.2155670
H	1.5546830	-3.8627200	-1.6920990	H	0.3563750	0.9417720	5.2562430
H	-2.8547810	-1.6936980	-1.0412520	H	2.2800090	0.4931670	3.7224670
C	-1.0713240	2.3396240	-0.4878890	H	-2.3631590	0.1979690	2.0005830
C	0.0475590	2.8306920	0.1867890	C	-2.1492800	1.3880060	-0.7198150
C	-1.8094070	3.1535340	-1.3516190	C	-1.2168200	2.4207200	-0.5103400
C	0.4274580	4.1594330	-0.0176180	C	-3.4339330	1.7249770	-1.1863220
H	0.5982290	2.2050840	0.8818070	C	-1.5623200	3.7417380	-0.7937020
C	-1.4183300	4.4775240	-1.5452710	H	-0.2247870	2.2145400	-0.1258540
H	-2.6679790	2.7403930	-1.8723900	C	-3.7585340	3.0489050	-1.4731930
C	-0.2991140	4.9821660	-0.8789300	H	-4.1961340	0.9603840	-1.2896870
H	1.2909610	4.5490520	0.5133810	C	-2.8261890	4.0691610	-1.2839850
H	-1.9858920	5.1107340	-2.2210990	H	-0.8221640	4.5201180	-0.6284300
H	0.0029110	6.0147940	-1.0288670	H	-4.7574870	3.2801920	-1.8338160
C	3.6859550	-0.6542180	0.0206080	H	-3.0842720	5.1009910	-1.5035200
C	4.1536690	-0.0634150	-1.1626110	C	3.9320980	0.2962960	-0.2041010
C	4.4112170	-0.5086060	1.2122560	C	4.4780040	-0.9750780	0.0267350
C	5.3428580	0.6624680	-1.1501520	C	4.5607520	1.1759360	-1.0975460
H	3.5908830	-0.1802880	-2.0820020	C	5.6418910	-1.3598070	-0.6357540
C	5.5946430	0.2239980	1.2193110	H	3.9935680	-1.6495780	0.7237880
H	4.0264890	-0.9650020	2.1177580	C	5.7223300	0.7856850	-1.7575170
C	6.0624340	0.8074720	0.0387450	H	4.1227810	2.1549640	-1.2610240
H	5.7085030	1.1153330	-2.0674190	C	6.2633430	-0.4822980	-1.5276870
H	6.1510400	0.3428070	2.1444690	H	6.0651150	-2.3439500	-0.4558350
H	6.9879130	1.3771550	0.0453950	H	6.2055890	1.4672200	-2.4516270
C	0.5821530	-3.4067250	-1.5390070	H	7.1699880	-0.7865680	-2.0437200
C	-1.8262870	-3.5105160	-1.4875260	C	-0.4151050	-1.8704290	-0.2160750
C	0.2460820	0.2200240	2.5029720	C	-1.3305560	-2.0589730	-1.4644670
N	1.0435810	0.9613500	2.9310590	C	-0.8974600	-2.7155600	0.8827310
C	-3.0152240	-1.4758260	2.0115620	N	-1.2881260	-3.4273950	1.7119280
N	-3.7619310	-2.3668020	1.9775220	C	-0.5996320	-1.7424620	-2.6954080
H	-2.3975570	0.4025880	2.7671610	N	-0.0091720	-1.4994370	-3.6646910
H	-0.3718030	-1.6368650	1.6601680	H	0.6218760	-2.1476520	-0.4246640
				H	-1.7162140	-3.0784930	-1.5409830
<p>TS Ylide S-3' (X=Y=H) + fumaronitrile → (2<i>RS</i>,3<i>SR</i>,4<i>SR</i>, 5<i>SR</i>)-3,4-dicyano-1,5-diphenylpyrrolidine-2-carboxylic acid</p> 				<p><i>endo</i>-2-adduct (X=Y=H)</p> 			
<p>E = -1467.25024914, H (0K) = -1466.856130, H (298K) = -1466.826774, G (298K) = -1466.918198 au.</p>				<p>E = -1204.21405519, H (0K) = -1203.868843, H (298K) = -1203.847236, G (298K) = -1203.920199 au.</p>			
<p>Imaginary frequency = 1.</p>				<p>Imaginary frequency = 0.</p>			
C	-0.7170410	-1.4036300	-0.9619900	C	1.0831500	4.6083060	-0.2881830
C	0.5167780	-2.0688940	-1.1853280	C	-0.1935770	4.6051120	-0.8563310
C	-0.6251740	0.0091550	-0.6226230	C	-0.8182630	3.3905360	-1.1423530
O	2.0654980	-2.1182230	1.0123750	C	-0.1821950	2.1842510	-0.8556220
C	2.4369950	-1.4517710	0.0742000	C	1.0943300	2.2056390	-0.2800660
				C	1.7369940	3.4102560	-0.0017590

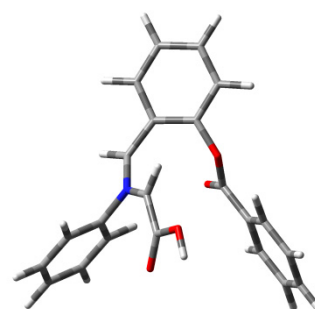
O	1.7076150	-1.3439830	-1.0959030	C	-0.7628200	0.8203030	-1.1520880
N	-1.5293840	0.9612850	-0.3256930	O	0.3520120	-0.0309620	-1.5175980
C	-2.7081460	0.8349580	0.4301950	C	1.0336370	-0.1702800	-0.2947430
C	-3.9647110	0.3416480	-0.1592450	O	1.7545830	1.0328440	0.0152420
O	-4.1393430	-0.1278900	-1.2708340	N	-1.3189880	0.2000170	0.0375590
O	-4.9797290	0.5232020	0.7233850	C	-0.1648150	-0.3650220	0.7415950
H	0.3248920	0.4454950	-0.9071200	C	0.1018710	0.2622900	2.1062300
H	-2.8984280	1.7622370	0.9639110	O	-0.4988960	1.1828120	2.6047760
H	-5.7734010	0.1374380	0.3090840	O	1.1078480	-0.3942900	2.7345510
C	-2.0958020	-0.3667480	2.0611760	H	1.5773780	5.5503430	-0.0670800
C	-1.8895500	-2.1650500	-1.1374760	H	-0.6956470	5.5414810	-1.0805120
C	-0.7180460	-0.6561300	1.9568580	H	-1.8081880	3.3764330	-1.5930000
H	-2.7507020	-4.0660880	-1.6112280	H	2.7310080	3.3932610	0.4339460
C	-0.5969170	-4.1386470	-1.6864930	H	-1.4756550	0.8439720	-1.9747960
H	-0.5505210	-5.1892360	-1.9574110	H	-0.3040580	-1.4391660	0.8994110
H	1.5546830	-3.8627200	-1.6920990	H	1.2307710	0.0550920	3.5920630
H	-2.8547810	-1.6936980	-1.0412520	C	-2.4904240	-0.6077880	-0.0437230
C	-1.0713240	2.3396240	-0.4878890	C	-3.2215520	-0.8089310	1.1370280
C	0.0475590	2.8306920	0.1867890	C	-2.9374520	-1.2047310	-1.2321600
C	-1.8094070	3.1535340	-1.3516190	C	-4.3704050	-1.5973610	1.1299020
C	0.4274580	4.1594330	-0.0176180	H	-2.8885160	-0.3161750	2.0455560
H	0.5982290	2.2050840	0.8818070	C	-4.1039140	-1.9715900	-1.2356440
C	-1.4183300	4.4775240	-1.5452710	H	-2.3674680	-1.0961000	-2.1499520
H	-2.6679790	2.7403930	-1.8723900	C	-4.8231230	-2.1765330	-0.0577720
C	-0.2991140	4.9821660	-0.8789300	H	-4.9253810	-1.7416100	2.0532170
H	1.2909610	4.5490520	0.5133810	H	-4.4388520	-2.4257340	-2.1646740
H	-1.9858920	5.1107340	-2.2210990	H	-5.7264630	-2.7798730	-0.0653010
H	0.0029110	6.0147940	-1.0288670	C	2.0194690	-1.3137530	-0.3585400
C	3.6859550	-0.6542180	0.0206080	C	3.2394030	-1.2559850	0.3224630
C	4.1536690	-0.0634150	-1.1626110	C	1.6898070	-2.4608960	-1.0904300
C	4.4112170	-0.5086060	1.2122560	C	4.1205130	-2.3365160	0.2688210
C	5.3428580	0.6624680	-1.1501520	H	3.4949460	-0.3675270	0.8869570
H	3.5908830	-0.1802880	-2.0820020	C	2.5736470	-3.5738720	-1.1419740
C	5.5946430	0.2239980	1.2193110	H	0.7483830	-2.4992860	-1.6288200
H	4.0264890	-0.9650020	2.1177580	C	3.7916410	-3.4789060	-0.4617950
C	6.0624340	0.8074720	0.0387450	H	5.0678860	-2.2824050	0.7984730
H	5.7085030	1.1153330	-2.0674190	H	2.3119370	-4.4211240	-1.7183770
H	6.1510400	0.3428070	2.1444690	H	4.4809160	-4.3181100	-0.5029210
H	6.9879130	1.3771550	0.0453950				
C	0.5821530	-3.4067250	-1.5390070				
C	-1.8262870	-3.5105160	-1.4875260				
C	0.2460820	0.2200240	2.5029720				
N	1.0435810	0.9613500	2.9310590				
C	-3.0152240	-1.4758260	2.0115620				
N	-3.7619310	-2.3668020	1.9775220				
H	-2.3975570	0.4025880	2.7671610				
H	-0.3718030	-1.6368650	1.6601680				

exo-2-adduct (X=Y=H)

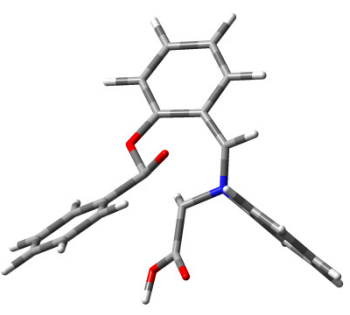
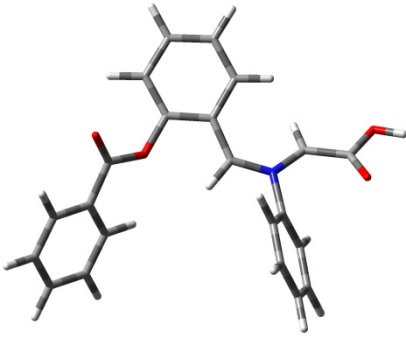


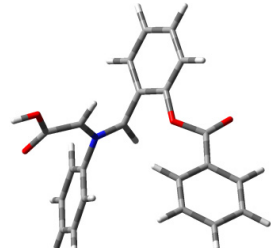
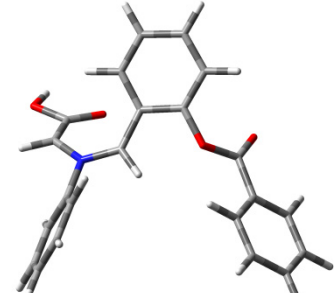
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 H (298K) = -1203.848749, G (298K) = -1203.921262

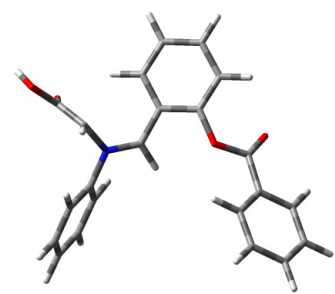
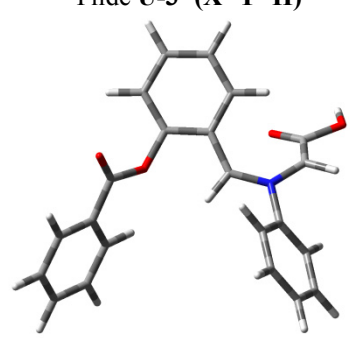
Ylide S-3 (X=Y=H)

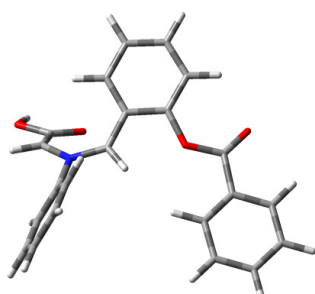
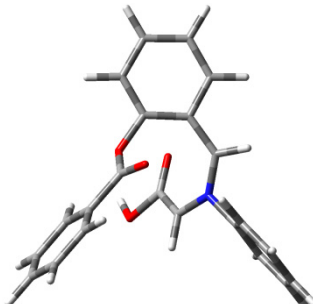


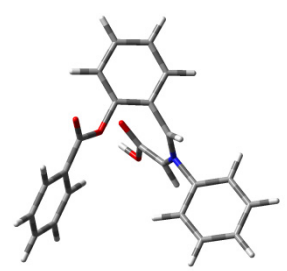
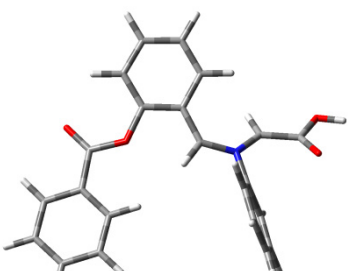
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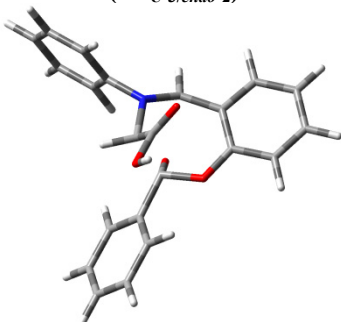
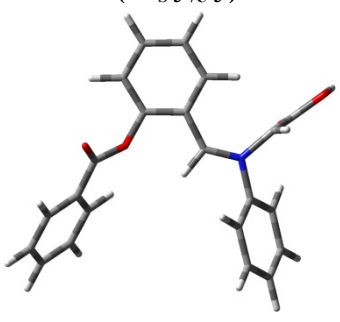
au.				au.			
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C	1.1529560	1.8467600	0.5709560	O	1.0414820	0.1481020	-1.9230870
C	0.2655930	2.2639580	-0.4327920	C	1.5124690	-0.3200800	-0.9104440
C	0.4951040	3.4360770	-1.1492440	O	1.9324300	0.4505920	0.1490960
C	0.7561330	0.5645210	1.2684230	N	-1.1770120	0.9304270	0.4482000
O	-0.6653880	0.6045920	1.4159730	C	-0.6134470	0.2919980	1.5157240
C	-1.1371590	0.3909290	0.1105650	C	-0.9142080	-1.0612110	1.8814750
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N	0.9468580	-0.6230110	0.4303980	O	-0.1488440	-1.4352360	2.9665300
C	-0.2307080	-0.7965320	-0.3959370	H	-1.3871670	2.5663450	-0.7518620
C	-0.8826320	-2.1643980	-0.1742530	H	0.1947840	0.8086140	2.0087850
O	-0.9018480	-2.7792900	0.8635950	H	-0.4133970	-2.3572810	3.1346690
O	-1.4657750	-2.6018630	-1.3167850	C	3.1058000	2.4893630	0.1667640
H	1.8215680	5.1021880	-1.4278560	C	3.1785410	3.8778710	0.0971270
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H	2.9503770	2.3169220	1.6491720	C	2.0053960	4.6167790	-0.0844400
H	-0.2154960	3.7409150	-1.9109400	C	0.7830180	3.9646920	-0.1594280
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H	-1.9095450	-3.4423690	-1.0943170	H	3.9987230	1.8817840	0.2755140
C	2.1831840	-1.1887970	0.1284860	C	-2.4868110	0.5151910	-0.0388580
C	2.3104340	-2.1327190	-0.9102500	C	-3.5743940	0.5104820	0.8325500
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C	3.5428200	-2.7223470	-1.1839360	C	-4.8326510	0.1785050	0.3381360
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H	-5.0929420	-1.0951980	2.0914390	H	2.8128430	-4.0032570	1.6702980
H	-5.3590390	0.4988720	-1.8959700	H	1.4740290	-4.7053630	-2.3596740
H	-6.4554090	-0.5154070	0.0928280	H	2.3382630	-5.5721570	-0.1960650
<p>TS Ylide S-3 (X=Y=H) → <i>exo</i>-2-adduct (X=Y=H) (TS_{S-3/exo-2})</p> 				<p>Ylide S-3' (X=Y=H)</p> 			
E = -1204.17330440, H (0K) = -1203.831209,				E = -1204.19794783, H (0K) = -1203.848416,			

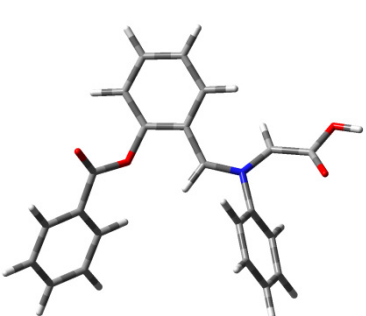
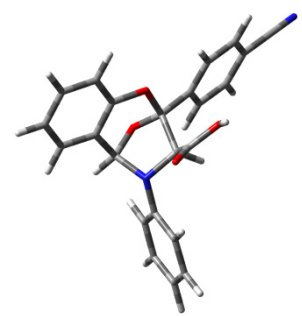
<p>H (298K) = -1203.809292, G (298K) = -1203.881700 au.</p> <p>Imaginary frequency = 1.</p> <table border="1"> <tbody> <tr><td>C</td><td>-0.8927330</td><td>-2.4660990</td><td>-0.2109690</td></tr> <tr><td>C</td><td>-2.0950560</td><td>-1.7420680</td><td>0.0303370</td></tr> <tr><td>C</td><td>0.4306190</td><td>-1.8903120</td><td>-0.3795710</td></tr> <tr><td>O</td><td>-0.4823430</td><td>-0.1430420</td><td>-1.5095080</td></tr> <tr><td>C</td><td>-0.9717210</td><td>0.3500810</td><td>-0.4429830</td></tr> <tr><td>O</td><td>-2.1812960</td><td>-0.4092730</td><td>0.0720970</td></tr> <tr><td>N</td><td>1.0170870</td><td>-0.9325100</td><td>0.3354940</td></tr> <tr><td>C</td><td>0.1219440</td><td>0.0300740</td><td>0.9207890</td></tr> <tr><td>C</td><td>0.7552070</td><td>1.2719110</td><td>1.4686890</td></tr> <tr><td>O</td><td>1.6730510</td><td>1.8993780</td><td>0.9891760</td></tr> <tr><td>O</td><td>0.0936460</td><td>1.6752830</td><td>2.5842550</td></tr> <tr><td>H</td><td>1.1328860</td><td>-2.4964110</td><td>-0.9452880</td></tr> <tr><td>H</td><td>-0.4962010</td><td>-0.4432460</td><td>1.6804840</td></tr> <tr><td>H</td><td>0.4577050</td><td>2.5527780</td><td>2.8073350</td></tr> <tr><td>C</td><td>-3.2935790</td><td>-2.4551210</td><td>0.2218090</td></tr> <tr><td>C</td><td>-3.3211750</td><td>-3.8381850</td><td>0.1464970</td></tr> <tr><td>H</td><td>-4.2617160</td><td>-4.3619370</td><td>0.2954720</td></tr> <tr><td>C</td><td>-2.1545060</td><td>-4.5616810</td><td>-0.1474650</td></tr> <tr><td>C</td><td>-0.9691970</td><td>-3.8737860</td><td>-0.3368690</td></tr> <tr><td>H</td><td>-2.1806950</td><td>-5.6435890</td><td>-0.2306530</td></tr> <tr><td>H</td><td>-0.0581080</td><td>-4.4214310</td><td>-0.5672560</td></tr> <tr><td>H</td><td>-4.1950960</td><td>-1.8797780</td><td>0.4056950</td></tr> <tr><td>C</td><td>2.4132180</td><td>-0.6570840</td><td>0.0438030</td></tr> <tr><td>C</td><td>3.3626990</td><td>-0.8710580</td><td>1.0417500</td></tr> <tr><td>C</td><td>2.7857560</td><td>-0.2393970</td><td>-1.2340110</td></tr> <tr><td>C</td><td>4.7112110</td><td>-0.6598880</td><td>0.7552350</td></tr> <tr><td>H</td><td>3.0464860</td><td>-1.2026300</td><td>2.0264770</td></tr> <tr><td>C</td><td>4.1376980</td><td>-0.0375220</td><td>-1.5111730</td></tr> <tr><td>H</td><td>2.0117320</td><td>-0.0569850</td><td>-1.9720420</td></tr> <tr><td>C</td><td>5.0995670</td><td>-0.2453840</td><td>-0.5204400</td></tr> <tr><td>H</td><td>5.4573670</td><td>-0.8254630</td><td>1.5271910</td></tr> <tr><td>H</td><td>4.4377990</td><td>0.2927120</td><td>-2.5016770</td></tr> <tr><td>H</td><td>6.1509290</td><td>-0.0828790</td><td>-0.7410320</td></tr> <tr><td>C</td><td>-1.3921810</td><td>1.8099620</td><td>-0.4512830</td></tr> <tr><td>C</td><td>-2.2875410</td><td>2.3359330</td><td>0.4876370</td></tr> <tr><td>C</td><td>-0.8529070</td><td>2.6495170</td><td>-1.4308670</td></tr> <tr><td>C</td><td>-2.6386300</td><td>3.6857930</td><td>0.4423450</td></tr> <tr><td>H</td><td>-2.7177750</td><td>1.6868970</td><td>1.2424760</td></tr> <tr><td>C</td><td>-1.1996700</td><td>3.9997430</td><td>-1.4702840</td></tr> <tr><td>H</td><td>-0.1722580</td><td>2.2259480</td><td>-2.1610010</td></tr> <tr><td>C</td><td>-2.0941070</td><td>4.5222090</td><td>-0.5342170</td></tr> <tr><td>H</td><td>-3.3426210</td><td>4.0828390</td><td>1.1695160</td></tr> <tr><td>H</td><td>-0.7752160</td><td>4.6426760</td><td>-2.2371000</td></tr> <tr><td>H</td><td>-2.3687770</td><td>5.5734750</td><td>-0.5677660</td></tr> </tbody> </table>	C	-0.8927330	-2.4660990	-0.2109690	C	-2.0950560	-1.7420680	0.0303370	C	0.4306190	-1.8903120	-0.3795710	O	-0.4823430	-0.1430420	-1.5095080	C	-0.9717210	0.3500810	-0.4429830	O	-2.1812960	-0.4092730	0.0720970	N	1.0170870	-0.9325100	0.3354940	C	0.1219440	0.0300740	0.9207890	C	0.7552070	1.2719110	1.4686890	O	1.6730510	1.8993780	0.9891760	O	0.0936460	1.6752830	2.5842550	H	1.1328860	-2.4964110	-0.9452880	H	-0.4962010	-0.4432460	1.6804840	H	0.4577050	2.5527780	2.8073350	C	-3.2935790	-2.4551210	0.2218090	C	-3.3211750	-3.8381850	0.1464970	H	-4.2617160	-4.3619370	0.2954720	C	-2.1545060	-4.5616810	-0.1474650	C	-0.9691970	-3.8737860	-0.3368690	H	-2.1806950	-5.6435890	-0.2306530	H	-0.0581080	-4.4214310	-0.5672560	H	-4.1950960	-1.8797780	0.4056950	C	2.4132180	-0.6570840	0.0438030	C	3.3626990	-0.8710580	1.0417500	C	2.7857560	-0.2393970	-1.2340110	C	4.7112110	-0.6598880	0.7552350	H	3.0464860	-1.2026300	2.0264770	C	4.1376980	-0.0375220	-1.5111730	H	2.0117320	-0.0569850	-1.9720420	C	5.0995670	-0.2453840	-0.5204400	H	5.4573670	-0.8254630	1.5271910	H	4.4377990	0.2927120	-2.5016770	H	6.1509290	-0.0828790	-0.7410320	C	-1.3921810	1.8099620	-0.4512830	C	-2.2875410	2.3359330	0.4876370	C	-0.8529070	2.6495170	-1.4308670	C	-2.6386300	3.6857930	0.4423450	H	-2.7177750	1.6868970	1.2424760	C	-1.1996700	3.9997430	-1.4702840	H	-0.1722580	2.2259480	-2.1610010	C	-2.0941070	4.5222090	-0.5342170	H	-3.3426210	4.0828390	1.1695160	H	-0.7752160	4.6426760	-2.2371000	H	-2.3687770	5.5734750	-0.5677660	<p>H (298K) = -1203.825450, G (298K) = -1203.912177 au.</p> <p>Imaginary frequency = 0.</p> <table border="1"> <tbody> <tr><td>C</td><td>0.3790010</td><td>1.9039310</td><td>0.0010860</td></tr> <tr><td>C</td><td>-1.0117650</td><td>2.1675210</td><td>-0.0992140</td></tr> <tr><td>C</td><td>0.8023040</td><td>0.5229350</td><td>0.0250370</td></tr> <tr><td>O</td><td>-3.3059990</td><td>1.5591400</td><td>1.3264030</td></tr> <tr><td>C</td><td>-2.9705880</td><td>0.8558100</td><td>0.4015610</td></tr> <tr><td>O</td><td>-1.8377170</td><td>1.0714490</td><td>-0.3499780</td></tr> <tr><td>N</td><td>2.0391800</td><td>0.0274200</td><td>-0.1330670</td></tr> <tr><td>C</td><td>3.1089060</td><td>0.6940840</td><td>-0.6648470</td></tr> <tr><td>C</td><td>4.4721740</td><td>0.3385520</td><td>-0.3998850</td></tr> <tr><td>O</td><td>4.9135760</td><td>-0.5397910</td><td>0.3326420</td></tr> <tr><td>O</td><td>5.3207190</td><td>1.1670610</td><td>-1.1004280</td></tr> <tr><td>H</td><td>0.0403230</td><td>-0.2287010</td><td>0.1654020</td></tr> <tr><td>H</td><td>2.8897430</td><td>1.5811150</td><td>-1.2373220</td></tr> <tr><td>H</td><td>6.2119350</td><td>0.8700260</td><td>-0.8438630</td></tr> <tr><td>C</td><td>-1.5313040</td><td>3.4545090</td><td>-0.0388580</td></tr> <tr><td>C</td><td>-0.6700750</td><td>4.5358590</td><td>0.1437350</td></tr> <tr><td>H</td><td>-1.0729560</td><td>5.5432960</td><td>0.1867700</td></tr> <tr><td>C</td><td>0.7042070</td><td>4.3148870</td><td>0.2609440</td></tr> <tr><td>C</td><td>1.2218950</td><td>3.0283890</td><td>0.1754520</td></tr> <tr><td>H</td><td>1.3805450</td><td>5.1516930</td><td>0.4099470</td></tr> <tr><td>H</td><td>2.2902390</td><td>2.8819640</td><td>0.2742150</td></tr> <tr><td>H</td><td>-2.6001240</td><td>3.6039120</td><td>-0.1296420</td></tr> <tr><td>C</td><td>2.1778660</td><td>-1.3851780</td><td>0.2027130</td></tr> <tr><td>C</td><td>1.8075460</td><td>-1.8233210</td><td>1.4718670</td></tr> <tr><td>C</td><td>2.6199480</td><td>-2.2790830</td><td>-0.7716740</td></tr> <tr><td>C</td><td>1.8875330</td><td>-3.1839920</td><td>1.7720570</td></tr> <tr><td>H</td><td>1.4843980</td><td>-1.1033890</td><td>2.2169170</td></tr> <tr><td>C</td><td>2.6910370</td><td>-3.6347720</td><td>-0.4642280</td></tr> <tr><td>H</td><td>2.9002670</td><td>-1.9069020</td><td>-1.7514840</td></tr> <tr><td>C</td><td>2.3273050</td><td>-4.0896740</td><td>0.8067170</td></tr> <tr><td>H</td><td>1.6121000</td><td>-3.5312040</td><td>2.7636730</td></tr> <tr><td>H</td><td>3.0302390</td><td>-4.3384550</td><td>-1.2189770</td></tr> <tr><td>H</td><td>2.3896270</td><td>-5.1482630</td><td>1.0428010</td></tr> <tr><td>C</td><td>-3.7083260</td><td>-0.3473870</td><td>-0.0674270</td></tr> <tr><td>C</td><td>-3.2959200</td><td>-1.1090700</td><td>-1.1707350</td></tr> <tr><td>C</td><td>-4.8636930</td><td>-0.7117990</td><td>0.6393470</td></tr> <tr><td>C</td><td>-4.0353600</td><td>-2.2251340</td><td>-1.5580850</td></tr> <tr><td>H</td><td>-2.4048540</td><td>-0.8235930</td><td>-1.7181120</td></tr> <tr><td>C</td><td>-5.5979170</td><td>-1.8279170</td><td>0.2487500</td></tr> <tr><td>H</td><td>-5.1669030</td><td>-0.1083310</td><td>1.4884990</td></tr> <tr><td>C</td><td>-5.1845190</td><td>-2.5857660</td><td>-0.8503890</td></tr> <tr><td>H</td><td>-3.7150080</td><td>-2.8136880</td><td>-2.4131610</td></tr> <tr><td>H</td><td>-6.4918720</td><td>-2.1077580</td><td>0.7988990</td></tr> <tr><td>H</td><td>-5.7581340</td><td>-3.4568450</td><td>-1.1557400</td></tr> </tbody> </table>	C	0.3790010	1.9039310	0.0010860	C	-1.0117650	2.1675210	-0.0992140	C	0.8023040	0.5229350	0.0250370	O	-3.3059990	1.5591400	1.3264030	C	-2.9705880	0.8558100	0.4015610	O	-1.8377170	1.0714490	-0.3499780	N	2.0391800	0.0274200	-0.1330670	C	3.1089060	0.6940840	-0.6648470	C	4.4721740	0.3385520	-0.3998850	O	4.9135760	-0.5397910	0.3326420	O	5.3207190	1.1670610	-1.1004280	H	0.0403230	-0.2287010	0.1654020	H	2.8897430	1.5811150	-1.2373220	H	6.2119350	0.8700260	-0.8438630	C	-1.5313040	3.4545090	-0.0388580	C	-0.6700750	4.5358590	0.1437350	H	-1.0729560	5.5432960	0.1867700	C	0.7042070	4.3148870	0.2609440	C	1.2218950	3.0283890	0.1754520	H	1.3805450	5.1516930	0.4099470	H	2.2902390	2.8819640	0.2742150	H	-2.6001240	3.6039120	-0.1296420	C	2.1778660	-1.3851780	0.2027130	C	1.8075460	-1.8233210	1.4718670	C	2.6199480	-2.2790830	-0.7716740	C	1.8875330	-3.1839920	1.7720570	H	1.4843980	-1.1033890	2.2169170	C	2.6910370	-3.6347720	-0.4642280	H	2.9002670	-1.9069020	-1.7514840	C	2.3273050	-4.0896740	0.8067170	H	1.6121000	-3.5312040	2.7636730	H	3.0302390	-4.3384550	-1.2189770	H	2.3896270	-5.1482630	1.0428010	C	-3.7083260	-0.3473870	-0.0674270	C	-3.2959200	-1.1090700	-1.1707350	C	-4.8636930	-0.7117990	0.6393470	C	-4.0353600	-2.2251340	-1.5580850	H	-2.4048540	-0.8235930	-1.7181120	C	-5.5979170	-1.8279170	0.2487500	H	-5.1669030	-0.1083310	1.4884990	C	-5.1845190	-2.5857660	-0.8503890	H	-3.7150080	-2.8136880	-2.4131610	H	-6.4918720	-2.1077580	0.7988990	H	-5.7581340	-3.4568450	-1.1557400
C	-0.8927330	-2.4660990	-0.2109690																																																																																																																																																																																																																																																																																																																																																														
C	-2.0950560	-1.7420680	0.0303370																																																																																																																																																																																																																																																																																																																																																														
C	0.4306190	-1.8903120	-0.3795710																																																																																																																																																																																																																																																																																																																																																														
O	-0.4823430	-0.1430420	-1.5095080																																																																																																																																																																																																																																																																																																																																																														
C	-0.9717210	0.3500810	-0.4429830																																																																																																																																																																																																																																																																																																																																																														
O	-2.1812960	-0.4092730	0.0720970																																																																																																																																																																																																																																																																																																																																																														
N	1.0170870	-0.9325100	0.3354940																																																																																																																																																																																																																																																																																																																																																														
C	0.1219440	0.0300740	0.9207890																																																																																																																																																																																																																																																																																																																																																														
C	0.7552070	1.2719110	1.4686890																																																																																																																																																																																																																																																																																																																																																														
O	1.6730510	1.8993780	0.9891760																																																																																																																																																																																																																																																																																																																																																														
O	0.0936460	1.6752830	2.5842550																																																																																																																																																																																																																																																																																																																																																														
H	1.1328860	-2.4964110	-0.9452880																																																																																																																																																																																																																																																																																																																																																														
H	-0.4962010	-0.4432460	1.6804840																																																																																																																																																																																																																																																																																																																																																														
H	0.4577050	2.5527780	2.8073350																																																																																																																																																																																																																																																																																																																																																														
C	-3.2935790	-2.4551210	0.2218090																																																																																																																																																																																																																																																																																																																																																														
C	-3.3211750	-3.8381850	0.1464970																																																																																																																																																																																																																																																																																																																																																														
H	-4.2617160	-4.3619370	0.2954720																																																																																																																																																																																																																																																																																																																																																														
C	-2.1545060	-4.5616810	-0.1474650																																																																																																																																																																																																																																																																																																																																																														
C	-0.9691970	-3.8737860	-0.3368690																																																																																																																																																																																																																																																																																																																																																														
H	-2.1806950	-5.6435890	-0.2306530																																																																																																																																																																																																																																																																																																																																																														
H	-0.0581080	-4.4214310	-0.5672560																																																																																																																																																																																																																																																																																																																																																														
H	-4.1950960	-1.8797780	0.4056950																																																																																																																																																																																																																																																																																																																																																														
C	2.4132180	-0.6570840	0.0438030																																																																																																																																																																																																																																																																																																																																																														
C	3.3626990	-0.8710580	1.0417500																																																																																																																																																																																																																																																																																																																																																														
C	2.7857560	-0.2393970	-1.2340110																																																																																																																																																																																																																																																																																																																																																														
C	4.7112110	-0.6598880	0.7552350																																																																																																																																																																																																																																																																																																																																																														
H	3.0464860	-1.2026300	2.0264770																																																																																																																																																																																																																																																																																																																																																														
C	4.1376980	-0.0375220	-1.5111730																																																																																																																																																																																																																																																																																																																																																														
H	2.0117320	-0.0569850	-1.9720420																																																																																																																																																																																																																																																																																																																																																														
C	5.0995670	-0.2453840	-0.5204400																																																																																																																																																																																																																																																																																																																																																														
H	5.4573670	-0.8254630	1.5271910																																																																																																																																																																																																																																																																																																																																																														
H	4.4377990	0.2927120	-2.5016770																																																																																																																																																																																																																																																																																																																																																														
H	6.1509290	-0.0828790	-0.7410320																																																																																																																																																																																																																																																																																																																																																														
C	-1.3921810	1.8099620	-0.4512830																																																																																																																																																																																																																																																																																																																																																														
C	-2.2875410	2.3359330	0.4876370																																																																																																																																																																																																																																																																																																																																																														
C	-0.8529070	2.6495170	-1.4308670																																																																																																																																																																																																																																																																																																																																																														
C	-2.6386300	3.6857930	0.4423450																																																																																																																																																																																																																																																																																																																																																														
H	-2.7177750	1.6868970	1.2424760																																																																																																																																																																																																																																																																																																																																																														
C	-1.1996700	3.9997430	-1.4702840																																																																																																																																																																																																																																																																																																																																																														
H	-0.1722580	2.2259480	-2.1610010																																																																																																																																																																																																																																																																																																																																																														
C	-2.0941070	4.5222090	-0.5342170																																																																																																																																																																																																																																																																																																																																																														
H	-3.3426210	4.0828390	1.1695160																																																																																																																																																																																																																																																																																																																																																														
H	-0.7752160	4.6426760	-2.2371000																																																																																																																																																																																																																																																																																																																																																														
H	-2.3687770	5.5734750	-0.5677660																																																																																																																																																																																																																																																																																																																																																														
C	0.3790010	1.9039310	0.0010860																																																																																																																																																																																																																																																																																																																																																														
C	-1.0117650	2.1675210	-0.0992140																																																																																																																																																																																																																																																																																																																																																														
C	0.8023040	0.5229350	0.0250370																																																																																																																																																																																																																																																																																																																																																														
O	-3.3059990	1.5591400	1.3264030																																																																																																																																																																																																																																																																																																																																																														
C	-2.9705880	0.8558100	0.4015610																																																																																																																																																																																																																																																																																																																																																														
O	-1.8377170	1.0714490	-0.3499780																																																																																																																																																																																																																																																																																																																																																														
N	2.0391800	0.0274200	-0.1330670																																																																																																																																																																																																																																																																																																																																																														
C	3.1089060	0.6940840	-0.6648470																																																																																																																																																																																																																																																																																																																																																														
C	4.4721740	0.3385520	-0.3998850																																																																																																																																																																																																																																																																																																																																																														
O	4.9135760	-0.5397910	0.3326420																																																																																																																																																																																																																																																																																																																																																														
O	5.3207190	1.1670610	-1.1004280																																																																																																																																																																																																																																																																																																																																																														
H	0.0403230	-0.2287010	0.1654020																																																																																																																																																																																																																																																																																																																																																														
H	2.8897430	1.5811150	-1.2373220																																																																																																																																																																																																																																																																																																																																																														
H	6.2119350	0.8700260	-0.8438630																																																																																																																																																																																																																																																																																																																																																														
C	-1.5313040	3.4545090	-0.0388580																																																																																																																																																																																																																																																																																																																																																														
C	-0.6700750	4.5358590	0.1437350																																																																																																																																																																																																																																																																																																																																																														
H	-1.0729560	5.5432960	0.1867700																																																																																																																																																																																																																																																																																																																																																														
C	0.7042070	4.3148870	0.2609440																																																																																																																																																																																																																																																																																																																																																														
C	1.2218950	3.0283890	0.1754520																																																																																																																																																																																																																																																																																																																																																														
H	1.3805450	5.1516930	0.4099470																																																																																																																																																																																																																																																																																																																																																														
H	2.2902390	2.8819640	0.2742150																																																																																																																																																																																																																																																																																																																																																														
H	-2.6001240	3.6039120	-0.1296420																																																																																																																																																																																																																																																																																																																																																														
C	2.1778660	-1.3851780	0.2027130																																																																																																																																																																																																																																																																																																																																																														
C	1.8075460	-1.8233210	1.4718670																																																																																																																																																																																																																																																																																																																																																														
C	2.6199480	-2.2790830	-0.7716740																																																																																																																																																																																																																																																																																																																																																														
C	1.8875330	-3.1839920	1.7720570																																																																																																																																																																																																																																																																																																																																																														
H	1.4843980	-1.1033890	2.2169170																																																																																																																																																																																																																																																																																																																																																														
C	2.6910370	-3.6347720	-0.4642280																																																																																																																																																																																																																																																																																																																																																														
H	2.9002670	-1.9069020	-1.7514840																																																																																																																																																																																																																																																																																																																																																														
C	2.3273050	-4.0896740	0.8067170																																																																																																																																																																																																																																																																																																																																																														
H	1.6121000	-3.5312040	2.7636730																																																																																																																																																																																																																																																																																																																																																														
H	3.0302390	-4.3384550	-1.2189770																																																																																																																																																																																																																																																																																																																																																														
H	2.3896270	-5.1482630	1.0428010																																																																																																																																																																																																																																																																																																																																																														
C	-3.7083260	-0.3473870	-0.0674270																																																																																																																																																																																																																																																																																																																																																														
C	-3.2959200	-1.1090700	-1.1707350																																																																																																																																																																																																																																																																																																																																																														
C	-4.8636930	-0.7117990	0.6393470																																																																																																																																																																																																																																																																																																																																																														
C	-4.0353600	-2.2251340	-1.5580850																																																																																																																																																																																																																																																																																																																																																														
H	-2.4048540	-0.8235930	-1.7181120																																																																																																																																																																																																																																																																																																																																																														
C	-5.5979170	-1.8279170	0.2487500																																																																																																																																																																																																																																																																																																																																																														
H	-5.1669030	-0.1083310	1.4884990																																																																																																																																																																																																																																																																																																																																																														
C	-5.1845190	-2.5857660	-0.8503890																																																																																																																																																																																																																																																																																																																																																														
H	-3.7150080	-2.8136880	-2.4131610																																																																																																																																																																																																																																																																																																																																																														
H	-6.4918720	-2.1077580	0.7988990																																																																																																																																																																																																																																																																																																																																																														
H	-5.7581340	-3.4568450	-1.1557400																																																																																																																																																																																																																																																																																																																																																														
<p>TS Ylide S-3 (X=Y=H) → Ylide S-3' (X=Y=H) (TS_{S-3/S-3'})</p>  <p>E = -1204.18947728, H (0K) = -1203.848416,</p>	<p>Ylide U-3'' (X=Y=H)</p>  <p>E = -1204.19725939, H (0K) = -1203.855022,</p>																																																																																																																																																																																																																																																																																																																																																																

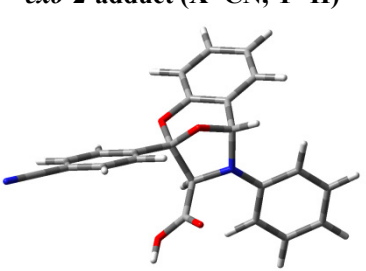
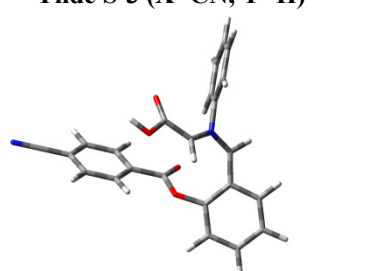
H (298K) = -1203.825450, G (298K) = -1203.903111 au.				H (298K) = -1203.831618, G (298K) = -1203.910167 au.			
Imaginary frequency = 1.				Imaginary frequency = 0.			
C	-0.1220610	2.2081840	-0.5980360	C	-0.7534880	-1.5449400	-0.5960940
C	1.2065170	2.0906180	-0.1617270	C	0.5976130	-1.9411430	-0.7677110
C	-0.9211270	1.0147560	-0.9503110	C	-1.0109030	-0.1614440	-0.2949500
O	3.5182750	1.0275700	-1.2236260	O	2.7337210	-2.1571070	0.9600530
C	2.8472990	0.3622140	-0.4680360	C	2.6084310	-1.1586650	0.2913400
O	1.6673700	0.7989940	0.0836330	O	1.5774630	-0.9592030	-0.5975510
N	-1.6940610	0.3730190	-0.0751610	N	-2.1697030	0.4595690	-0.0271470
C	-1.7572100	0.6359400	1.2640850	C	-3.3469550	-0.0698840	0.4543420
C	-2.8426050	0.2173060	2.1001510	C	-3.3744700	-1.1448070	1.3902940
O	-3.8434350	-0.4314680	1.8130930	O	-2.4231040	-1.7876200	1.8269120
O	-2.6381180	0.6551870	3.3901140	O	-4.6618170	-1.4126170	1.8034950
H	-0.8298570	0.5565820	-1.9264920	H	-0.1668670	0.5103820	-0.3571550
H	-1.0253760	1.3304630	1.6467820	H	-4.2325530	0.5225040	0.2816090
H	-3.4208040	0.3388180	3.8753960	H	-4.5592300	-2.1284270	2.4555640
C	1.9927450	3.2088650	0.1093090	C	0.9505290	-3.2185280	-1.1783910
C	1.4422550	4.4793710	-0.0501720	C	-1.7385280	-2.5237800	-0.8618900
H	2.0512100	5.3544720	0.1582150	C	-1.3914050	-3.7965380	-1.2978640
C	0.1186950	4.6280700	-0.4693940	H	-2.1740810	-4.5206250	-1.5050630
C	-0.6533070	3.4997360	-0.7397340	C	-0.0497190	-4.1546450	-1.4427370
H	-0.3095880	5.6189560	-0.5887530	H	0.2225640	-5.1588360	-1.7543290
H	-1.6816590	3.6065020	-1.0729190	H	1.9980390	-3.4747180	-1.2840330
H	3.0174580	3.0815190	0.4374180	H	-2.7829590	-2.2622660	-0.7602810
C	-2.4516000	-0.7454780	-0.6320170	C	-2.1758470	1.8961420	-0.2466710
C	-3.3836540	-0.4992880	-1.6352940	C	-2.6503100	2.7441980	0.7562920
C	-2.1722000	-2.0400580	-0.2003250	C	-1.7156970	2.4105670	-1.4603490
C	-4.0587750	-1.5756700	-2.2135500	C	-2.6514750	4.1214460	0.5418100
H	-3.5877870	0.5215800	-1.9414840	H	-2.9956950	2.3198160	1.6931670
C	-2.8455260	-3.1073990	-0.7884320	C	-1.7230820	3.7905720	-1.6664810
H	-1.4392370	-2.1976800	0.5836740	H	-1.3791630	1.7312550	-2.2372230
C	-3.7901770	-2.8779780	-1.7928940	C	-2.1894740	4.6468530	-0.6677880
H	-4.7965910	-1.3917270	-2.9891540	H	-3.0071820	4.7851010	1.3246440
H	-2.6324850	-4.1210430	-0.4614330	H	-1.3759620	4.1932820	-2.6137390
H	-4.3161070	-3.7144180	-2.2444970	H	-2.1966480	5.7206950	-0.8319570
C	3.1728060	-1.0176940	-0.0197780	C	3.5351360	0.0064170	0.3175460
C	2.3860910	-1.7150860	0.9090330	C	3.4078360	1.0988960	-0.5521960
C	4.3214570	-1.6187480	-0.5542490	C	4.5752950	-0.0179980	1.2575960
C	2.7512480	-3.0031590	1.2961980	C	4.3133560	2.1557920	-0.4770190
H	1.5009150	-1.2457580	1.3237010	H	2.6085880	1.1121610	-1.2845330
C	4.6792770	-2.9068900	-0.1663370	C	5.4749290	1.0418090	1.3315630
H	4.9172680	-1.0602890	-1.2687080	H	4.6577980	-0.8741640	1.9188590
C	3.8948060	-3.6000140	0.7596370	C	5.3450490	2.1299840	0.4643620
H	2.1442030	-3.5414380	2.0187310	H	4.2146550	3.0001320	-1.1536240
H	5.5690230	-3.3706320	-0.5828310	H	6.2773840	1.0205660	2.0635520
H	4.1753800	-4.6048890	1.0639910	H	6.0482110	2.9566910	0.5212820
TS Ylide S-3' (X=Y=H) → Ylide U-3'' (X=Y=H) (TS _{S-3'/U-3''})				Ylide U-3' (X=Y=H)			
							
E = -1204.16908149, H (0K) = -1203.828678,				E = -1204.19858783, H (0K) = -1203.856319,			

<p>H (298K) = -1203.805390, G (298K) = -1203.883949 au.</p> <p>Imaginary frequency = 1.</p> <table border="1"> <tbody> <tr><td>C</td><td>-0.5136010</td><td>-1.6916760</td><td>0.0988670</td></tr> <tr><td>C</td><td>0.8425710</td><td>-2.0598740</td><td>-0.0239730</td></tr> <tr><td>C</td><td>-0.8392030</td><td>-0.2817470</td><td>0.1744830</td></tr> <tr><td>O</td><td>3.3206380</td><td>-1.8080950</td><td>1.2011720</td></tr> <tr><td>C</td><td>2.9670520</td><td>-0.9846990</td><td>0.3907120</td></tr> <tr><td>O</td><td>1.7375150</td><td>-1.0164230</td><td>-0.2402730</td></tr> <tr><td>N</td><td>-1.9169020</td><td>0.3026160</td><td>-0.2722170</td></tr> <tr><td>C</td><td>-2.8929580</td><td>-0.3447110</td><td>-1.1258210</td></tr> <tr><td>C</td><td>-4.0472740</td><td>-0.8100470</td><td>-0.4941990</td></tr> <tr><td>O</td><td>-4.1927330</td><td>-1.0194320</td><td>0.7276130</td></tr> <tr><td>O</td><td>-5.0742930</td><td>-1.1298320</td><td>-1.3650340</td></tr> <tr><td>H</td><td>-0.1142330</td><td>0.3707840</td><td>0.6550190</td></tr> <tr><td>H</td><td>-2.8280120</td><td>-0.0783700</td><td>-2.1717750</td></tr> <tr><td>H</td><td>-5.7482250</td><td>-1.5161770</td><td>-0.7788310</td></tr> <tr><td>C</td><td>1.2288150</td><td>-3.3963590</td><td>-0.0423760</td></tr> <tr><td>C</td><td>0.2478010</td><td>-4.3784160</td><td>0.0993620</td></tr> <tr><td>H</td><td>0.5444790</td><td>-5.4236570</td><td>0.0911220</td></tr> <tr><td>C</td><td>-1.0976340</td><td>-4.0351180</td><td>0.2628790</td></tr> <tr><td>C</td><td>-1.4868830</td><td>-2.7005170</td><td>0.2561120</td></tr> <tr><td>H</td><td>-1.8446420</td><td>-4.8104580</td><td>0.4016110</td></tr> <tr><td>H</td><td>-2.5154440</td><td>-2.4123410</td><td>0.4499650</td></tr> <tr><td>H</td><td>2.2712890</td><td>-3.6616880</td><td>-0.1575130</td></tr> <tr><td>C</td><td>-2.1446220</td><td>1.6808850</td><td>0.1228350</td></tr> <tr><td>C</td><td>-1.9648460</td><td>2.0632350</td><td>1.4548900</td></tr> <tr><td>C</td><td>-2.5736260</td><td>2.6063890</td><td>-0.8324390</td></tr> <tr><td>C</td><td>-2.1896080</td><td>3.3902280</td><td>1.8255940</td></tr> <tr><td>H</td><td>-1.7051400</td><td>1.3188630</td><td>2.2010370</td></tr> <tr><td>C</td><td>-2.7796850</td><td>3.9300460</td><td>-0.4551190</td></tr> <tr><td>H</td><td>-2.7480970</td><td>2.2815890</td><td>-1.8518110</td></tr> <tr><td>C</td><td>-2.5878380</td><td>4.3266680</td><td>0.8726120</td></tr> <tr><td>H</td><td>-2.0700380</td><td>3.6827360</td><td>2.8648250</td></tr> <tr><td>H</td><td>-3.0998090</td><td>4.6538310</td><td>-1.1991320</td></tr> <tr><td>H</td><td>-2.7669890</td><td>5.3577460</td><td>1.1636670</td></tr> <tr><td>C</td><td>3.7660300</td><td>0.1877150</td><td>-0.0481530</td></tr> <tr><td>C</td><td>3.3271200</td><td>1.0785220</td><td>-1.0390750</td></tr> <tr><td>C</td><td>5.0111880</td><td>0.3855010</td><td>0.5674050</td></tr> <tr><td>C</td><td>4.1295700</td><td>2.1569770</td><td>-1.4058610</td></tr> <tr><td>H</td><td>2.3677390</td><td>0.9220380</td><td>-1.5187620</td></tr> <tr><td>C</td><td>5.8074260</td><td>1.4656960</td><td>0.1984020</td></tr> <tr><td>H</td><td>5.3338080</td><td>-0.3164780</td><td>1.3291450</td></tr> <tr><td>C</td><td>5.3673660</td><td>2.3523380</td><td>-0.7883380</td></tr> <tr><td>H</td><td>3.7895880</td><td>2.8450720</td><td>-2.1745190</td></tr> <tr><td>H</td><td>6.7703720</td><td>1.6170670</td><td>0.6776540</td></tr> <tr><td>H</td><td>5.9896970</td><td>3.1951650</td><td>-1.0767770</td></tr> </tbody> </table>	C	-0.5136010	-1.6916760	0.0988670	C	0.8425710	-2.0598740	-0.0239730	C	-0.8392030	-0.2817470	0.1744830	O	3.3206380	-1.8080950	1.2011720	C	2.9670520	-0.9846990	0.3907120	O	1.7375150	-1.0164230	-0.2402730	N	-1.9169020	0.3026160	-0.2722170	C	-2.8929580	-0.3447110	-1.1258210	C	-4.0472740	-0.8100470	-0.4941990	O	-4.1927330	-1.0194320	0.7276130	O	-5.0742930	-1.1298320	-1.3650340	H	-0.1142330	0.3707840	0.6550190	H	-2.8280120	-0.0783700	-2.1717750	H	-5.7482250	-1.5161770	-0.7788310	C	1.2288150	-3.3963590	-0.0423760	C	0.2478010	-4.3784160	0.0993620	H	0.5444790	-5.4236570	0.0911220	C	-1.0976340	-4.0351180	0.2628790	C	-1.4868830	-2.7005170	0.2561120	H	-1.8446420	-4.8104580	0.4016110	H	-2.5154440	-2.4123410	0.4499650	H	2.2712890	-3.6616880	-0.1575130	C	-2.1446220	1.6808850	0.1228350	C	-1.9648460	2.0632350	1.4548900	C	-2.5736260	2.6063890	-0.8324390	C	-2.1896080	3.3902280	1.8255940	H	-1.7051400	1.3188630	2.2010370	C	-2.7796850	3.9300460	-0.4551190	H	-2.7480970	2.2815890	-1.8518110	C	-2.5878380	4.3266680	0.8726120	H	-2.0700380	3.6827360	2.8648250	H	-3.0998090	4.6538310	-1.1991320	H	-2.7669890	5.3577460	1.1636670	C	3.7660300	0.1877150	-0.0481530	C	3.3271200	1.0785220	-1.0390750	C	5.0111880	0.3855010	0.5674050	C	4.1295700	2.1569770	-1.4058610	H	2.3677390	0.9220380	-1.5187620	C	5.8074260	1.4656960	0.1984020	H	5.3338080	-0.3164780	1.3291450	C	5.3673660	2.3523380	-0.7883380	H	3.7895880	2.8450720	-2.1745190	H	6.7703720	1.6170670	0.6776540	H	5.9896970	3.1951650	-1.0767770	<p>H (298K) = -1203.832922, G (298K) = -1203.911752 au.</p> <p>Imaginary frequency = 0.</p> <table border="1"> <tbody> <tr><td>C</td><td>0.8307230</td><td>-1.5896210</td><td>-0.2877150</td></tr> <tr><td>C</td><td>-0.4929330</td><td>-2.0911850</td><td>-0.2068320</td></tr> <tr><td>C</td><td>1.0174610</td><td>-0.1719380</td><td>-0.1283680</td></tr> <tr><td>O</td><td>-2.8376030</td><td>-1.5603630</td><td>-1.5700040</td></tr> <tr><td>C</td><td>-2.6275520</td><td>-1.0221530</td><td>-0.5072800</td></tr> <tr><td>O</td><td>-1.4805620</td><td>-1.2046290</td><td>0.2283190</td></tr> <tr><td>N</td><td>2.1504150</td><td>0.5451750</td><td>-0.0924640</td></tr> <tr><td>C</td><td>3.4227510</td><td>0.1321560</td><td>0.2387720</td></tr> <tr><td>C</td><td>3.6683440</td><td>-0.8520050</td><td>1.2398710</td></tr> <tr><td>O</td><td>2.8432220</td><td>-1.5103090</td><td>1.8692290</td></tr> <tr><td>O</td><td>5.0191690</td><td>-1.0051540</td><td>1.4671750</td></tr> <tr><td>H</td><td>0.1229120</td><td>0.4340040</td><td>-0.1043260</td></tr> <tr><td>H</td><td>4.2267760</td><td>0.7581840</td><td>-0.1170230</td></tr> <tr><td>H</td><td>5.0677970</td><td>-1.6667720</td><td>2.1798170</td></tr> <tr><td>C</td><td>-0.8017330</td><td>-3.4183480</td><td>-0.4694900</td></tr> <tr><td>C</td><td>1.8386410</td><td>-2.5152000</td><td>-0.6427410</td></tr> <tr><td>C</td><td>1.5300800</td><td>-3.8362470</td><td>-0.9420130</td></tr> <tr><td>H</td><td>2.3257940</td><td>-4.5175060</td><td>-1.2292820</td></tr> <tr><td>C</td><td>0.2152600</td><td>-4.2964960</td><td>-0.8443350</td></tr> <tr><td>H</td><td>-0.0210650</td><td>-5.3370140</td><td>-1.0469090</td></tr> <tr><td>H</td><td>-1.8279780</td><td>-3.7555130</td><td>-0.3857620</td></tr> <tr><td>H</td><td>2.8628050</td><td>-2.1758560</td><td>-0.7200170</td></tr> <tr><td>C</td><td>2.0130010</td><td>1.9548280</td><td>-0.4173070</td></tr> <tr><td>C</td><td>1.3182600</td><td>2.3333770</td><td>-1.5678280</td></tr> <tr><td>C</td><td>2.5828970</td><td>2.9139100</td><td>0.4230250</td></tr> <tr><td>C</td><td>1.1843610</td><td>3.6884140</td><td>-1.8724610</td></tr> <tr><td>H</td><td>0.9088260</td><td>1.5708120</td><td>-2.2228480</td></tr> <tr><td>C</td><td>2.4430000</td><td>4.2649530</td><td>0.1103760</td></tr> <tr><td>H</td><td>3.1116370</td><td>2.5940380</td><td>1.3147720</td></tr> <tr><td>C</td><td>1.7448430</td><td>4.6546500</td><td>-1.0356510</td></tr> <tr><td>H</td><td>0.6519990</td><td>3.9855510</td><td>-2.7713700</td></tr> <tr><td>H</td><td>2.8738480</td><td>5.0143780</td><td>0.7681020</td></tr> <tr><td>H</td><td>1.6414610</td><td>5.7088200</td><td>-1.2768590</td></tr> <tr><td>C</td><td>-3.5542520</td><td>-0.0727960</td><td>0.1666620</td></tr> <tr><td>C</td><td>-3.2874270</td><td>0.4783000</td><td>1.4286100</td></tr> <tr><td>C</td><td>-4.7366990</td><td>0.2657800</td><td>-0.5071380</td></tr> <tr><td>C</td><td>-4.1980180</td><td>1.3619340</td><td>2.0054960</td></tr> 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</table>	C	0.8307230	-1.5896210	-0.2877150	C	-0.4929330	-2.0911850	-0.2068320	C	1.0174610	-0.1719380	-0.1283680	O	-2.8376030	-1.5603630	-1.5700040	C	-2.6275520	-1.0221530	-0.5072800	O	-1.4805620	-1.2046290	0.2283190	N	2.1504150	0.5451750	-0.0924640	C	3.4227510	0.1321560	0.2387720	C	3.6683440	-0.8520050	1.2398710	O	2.8432220	-1.5103090	1.8692290	O	5.0191690	-1.0051540	1.4671750	H	0.1229120	0.4340040	-0.1043260	H	4.2267760	0.7581840	-0.1170230	H	5.0677970	-1.6667720	2.1798170	C	-0.8017330	-3.4183480	-0.4694900	C	1.8386410	-2.5152000	-0.6427410	C	1.5300800	-3.8362470	-0.9420130	H	2.3257940	-4.5175060	-1.2292820	C	0.2152600	-4.2964960	-0.8443350	H	-0.0210650	-5.3370140	-1.0469090	H	-1.8279780	-3.7555130	-0.3857620	H	2.8628050	-2.1758560	-0.7200170	C	2.0130010	1.9548280	-0.4173070	C	1.3182600	2.3333770	-1.5678280	C	2.5828970	2.9139100	0.4230250	C	1.1843610	3.6884140	-1.8724610	H	0.9088260	1.5708120	-2.2228480	C	2.4430000	4.2649530	0.1103760	H	3.1116370	2.5940380	1.3147720	C	1.7448430	4.6546500	-1.0356510	H	0.6519990	3.9855510	-2.7713700	H	2.8738480	5.0143780	0.7681020	H	1.6414610	5.7088200	-1.2768590	C	-3.5542520	-0.0727960	0.1666620	C	-3.2874270	0.4783000	1.4286100	C	-4.7366990	0.2657800	-0.5071380	C	-4.1980180	1.3619340	2.0054960	H	-2.3755110	0.2101010	1.9499010	C	-5.6416840	1.1502530	0.0728440	H	-4.9255390	-0.1744710	-1.4807110	C	-5.3731460	1.6994050	1.3297390	H	-3.9909650	1.7865150	2.9838090	H	-6.5562090	1.4113610	-0.4522560	H	-6.0803830	2.3889570	1.7830500
C	-0.5136010	-1.6916760	0.0988670																																																																																																																																																																																																																																																																																																																																																														
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H	2.2712890	-3.6616880	-0.1575130																																																																																																																																																																																																																																																																																																																																																														
C	-2.1446220	1.6808850	0.1228350																																																																																																																																																																																																																																																																																																																																																														
C	-1.9648460	2.0632350	1.4548900																																																																																																																																																																																																																																																																																																																																																														
C	-2.5736260	2.6063890	-0.8324390																																																																																																																																																																																																																																																																																																																																																														
C	-2.1896080	3.3902280	1.8255940																																																																																																																																																																																																																																																																																																																																																														
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H	-2.0700380	3.6827360	2.8648250																																																																																																																																																																																																																																																																																																																																																														
H	-3.0998090	4.6538310	-1.1991320																																																																																																																																																																																																																																																																																																																																																														
H	-2.7669890	5.3577460	1.1636670																																																																																																																																																																																																																																																																																																																																																														
C	3.7660300	0.1877150	-0.0481530																																																																																																																																																																																																																																																																																																																																																														
C	3.3271200	1.0785220	-1.0390750																																																																																																																																																																																																																																																																																																																																																														
C	5.0111880	0.3855010	0.5674050																																																																																																																																																																																																																																																																																																																																																														
C	4.1295700	2.1569770	-1.4058610																																																																																																																																																																																																																																																																																																																																																														
H	2.3677390	0.9220380	-1.5187620																																																																																																																																																																																																																																																																																																																																																														
C	5.8074260	1.4656960	0.1984020																																																																																																																																																																																																																																																																																																																																																														
H	5.3338080	-0.3164780	1.3291450																																																																																																																																																																																																																																																																																																																																																														
C	5.3673660	2.3523380	-0.7883380																																																																																																																																																																																																																																																																																																																																																														
H	3.7895880	2.8450720	-2.1745190																																																																																																																																																																																																																																																																																																																																																														
H	6.7703720	1.6170670	0.6776540																																																																																																																																																																																																																																																																																																																																																														
H	5.9896970	3.1951650	-1.0767770																																																																																																																																																																																																																																																																																																																																																														
C	0.8307230	-1.5896210	-0.2877150																																																																																																																																																																																																																																																																																																																																																														
C	-0.4929330	-2.0911850	-0.2068320																																																																																																																																																																																																																																																																																																																																																														
C	1.0174610	-0.1719380	-0.1283680																																																																																																																																																																																																																																																																																																																																																														
O	-2.8376030	-1.5603630	-1.5700040																																																																																																																																																																																																																																																																																																																																																														
C	-2.6275520	-1.0221530	-0.5072800																																																																																																																																																																																																																																																																																																																																																														
O	-1.4805620	-1.2046290	0.2283190																																																																																																																																																																																																																																																																																																																																																														
N	2.1504150	0.5451750	-0.0924640																																																																																																																																																																																																																																																																																																																																																														
C	3.4227510	0.1321560	0.2387720																																																																																																																																																																																																																																																																																																																																																														
C	3.6683440	-0.8520050	1.2398710																																																																																																																																																																																																																																																																																																																																																														
O	2.8432220	-1.5103090	1.8692290																																																																																																																																																																																																																																																																																																																																																														
O	5.0191690	-1.0051540	1.4671750																																																																																																																																																																																																																																																																																																																																																														
H	0.1229120	0.4340040	-0.1043260																																																																																																																																																																																																																																																																																																																																																														
H	4.2267760	0.7581840	-0.1170230																																																																																																																																																																																																																																																																																																																																																														
H	5.0677970	-1.6667720	2.1798170																																																																																																																																																																																																																																																																																																																																																														
C	-0.8017330	-3.4183480	-0.4694900																																																																																																																																																																																																																																																																																																																																																														
C	1.8386410	-2.5152000	-0.6427410																																																																																																																																																																																																																																																																																																																																																														
C	1.5300800	-3.8362470	-0.9420130																																																																																																																																																																																																																																																																																																																																																														
H	2.3257940	-4.5175060	-1.2292820																																																																																																																																																																																																																																																																																																																																																														
C	0.2152600	-4.2964960	-0.8443350																																																																																																																																																																																																																																																																																																																																																														
H	-0.0210650	-5.3370140	-1.0469090																																																																																																																																																																																																																																																																																																																																																														
H	-1.8279780	-3.7555130	-0.3857620																																																																																																																																																																																																																																																																																																																																																														
H	2.8628050	-2.1758560	-0.7200170																																																																																																																																																																																																																																																																																																																																																														
C	2.0130010	1.9548280	-0.4173070																																																																																																																																																																																																																																																																																																																																																														
C	1.3182600	2.3333770	-1.5678280																																																																																																																																																																																																																																																																																																																																																														
C	2.5828970	2.9139100	0.4230250																																																																																																																																																																																																																																																																																																																																																														
C	1.1843610	3.6884140	-1.8724610																																																																																																																																																																																																																																																																																																																																																														
H	0.9088260	1.5708120	-2.2228480																																																																																																																																																																																																																																																																																																																																																														
C	2.4430000	4.2649530	0.1103760																																																																																																																																																																																																																																																																																																																																																														
H	3.1116370	2.5940380	1.3147720																																																																																																																																																																																																																																																																																																																																																														
C	1.7448430	4.6546500	-1.0356510																																																																																																																																																																																																																																																																																																																																																														
H	0.6519990	3.9855510	-2.7713700																																																																																																																																																																																																																																																																																																																																																														
H	2.8738480	5.0143780	0.7681020																																																																																																																																																																																																																																																																																																																																																														
H	1.6414610	5.7088200	-1.2768590																																																																																																																																																																																																																																																																																																																																																														
C	-3.5542520	-0.0727960	0.1666620																																																																																																																																																																																																																																																																																																																																																														
C	-3.2874270	0.4783000	1.4286100																																																																																																																																																																																																																																																																																																																																																														
C	-4.7366990	0.2657800	-0.5071380																																																																																																																																																																																																																																																																																																																																																														
C	-4.1980180	1.3619340	2.0054960																																																																																																																																																																																																																																																																																																																																																														
H	-2.3755110	0.2101010	1.9499010																																																																																																																																																																																																																																																																																																																																																														
C	-5.6416840	1.1502530	0.0728440																																																																																																																																																																																																																																																																																																																																																														
H	-4.9255390	-0.1744710	-1.4807110																																																																																																																																																																																																																																																																																																																																																														
C	-5.3731460	1.6994050	1.3297390																																																																																																																																																																																																																																																																																																																																																														
H	-3.9909650	1.7865150	2.9838090																																																																																																																																																																																																																																																																																																																																																														
H	-6.5562090	1.4113610	-0.4522560																																																																																																																																																																																																																																																																																																																																																														
H	-6.0803830	2.3889570	1.7830500																																																																																																																																																																																																																																																																																																																																																														
<p>TS Ylide U-3'' (X=Y=H) → Ylide U-3' (X=Y=H) (TS_{U-3''/U-3'})</p>  <p>E = -1204.19571209, H (0K) = -1203.853556,</p>	<p>Ylide U-3 (X=Y=H)</p>  <p>E = -1204.19857552, H (0K) = -1203.856553,</p>																																																																																																																																																																																																																																																																																																																																																																

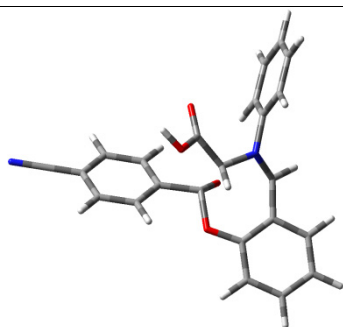
<p>H (298K) = -1203.831009, G (298K) = -1203.906425 au.</p> <p>Imaginary frequency = 1.</p> <table border="1"> <tbody> <tr><td>C</td><td>-0.6844280</td><td>-1.6240670</td><td>-0.4900170</td></tr> <tr><td>C</td><td>0.6847250</td><td>-2.0011690</td><td>-0.5865080</td></tr> <tr><td>C</td><td>-0.9967730</td><td>-0.2326310</td><td>-0.2898980</td></tr> <tr><td>O</td><td>3.4920240</td><td>-2.1828420</td><td>-0.0086960</td></tr> <tr><td>C</td><td>2.9088790</td><td>-1.1211150</td><td>-0.0342060</td></tr> <tr><td>O</td><td>1.5846530</td><td>-0.9643420</td><td>-0.3365220</td></tr> <tr><td>N</td><td>-2.1776940</td><td>0.3529610</td><td>-0.0406570</td></tr> <tr><td>C</td><td>-3.3178950</td><td>-0.1887890</td><td>0.5120560</td></tr> <tr><td>C</td><td>-3.2776900</td><td>-1.2071810</td><td>1.5082090</td></tr> <tr><td>O</td><td>-2.2903550</td><td>-1.7855790</td><td>1.9555810</td></tr> <tr><td>O</td><td>-4.5422950</td><td>-1.5008030</td><td>1.9710220</td></tr> <tr><td>H</td><td>-0.1937180</td><td>0.4723960</td><td>-0.4432110</td></tr> <tr><td>H</td><td>-4.2322240</td><td>0.3532570</td><td>0.3252490</td></tr> <tr><td>H</td><td>-4.3945660</td><td>-2.1730550</td><td>2.6597160</td></tr> <tr><td>C</td><td>1.0639260</td><td>-3.2904650</td><td>-0.9502620</td></tr> <tr><td>C</td><td>-1.6470360</td><td>-2.6261690</td><td>-0.7361410</td></tr> <tr><td>C</td><td>-1.2736260</td><td>-3.9093520</td><td>-1.1146140</td></tr> <tr><td>H</td><td>-2.0389020</td><td>-4.6540490</td><td>-1.3135080</td></tr> <tr><td>C</td><td>0.0765920</td><td>-4.2426650</td><td>-1.2143140</td></tr> <tr><td>H</td><td>0.3754300</td><td>-5.2508730</td><td>-1.4868890</td></tr> <tr><td>H</td><td>2.1099320</td><td>-3.5475580</td><td>-1.0096190</td></tr> <tr><td>H</td><td>-2.6970880</td><td>-2.3726610</td><td>-0.6684620</td></tr> <tr><td>C</td><td>-2.2577030</td><td>1.7663330</td><td>-0.3705570</td></tr> <tr><td>C</td><td>-2.7487840</td><td>2.6677110</td><td>0.5764920</td></tr> <tr><td>C</td><td>-1.8490550</td><td>2.2051510</td><td>-1.6314900</td></tr> <tr><td>C</td><td>-2.8188160</td><td>4.0227170</td><td>0.2572200</td></tr> <tr><td>H</td><td>-3.0543180</td><td>2.3019890</td><td>1.5511730</td></tr> <tr><td>C</td><td>-1.9248580</td><td>3.5634700</td><td>-1.9422910</td></tr> <tr><td>H</td><td>-1.4984070</td><td>1.4838220</td><td>-2.3629170</td></tr> <tr><td>C</td><td>-2.4082200</td><td>4.4729900</td><td>-1.0003830</td></tr> <tr><td>H</td><td>-3.1885340</td><td>4.7284490</td><td>0.9955360</td></tr> <tr><td>H</td><td>-1.6173760</td><td>3.9062280</td><td>-2.9260630</td></tr> <tr><td>H</td><td>-2.4689640</td><td>5.5294710</td><td>-1.2459370</td></tr> <tr><td>C</td><td>3.5599440</td><td>0.1886270</td><td>0.2545600</td></tr> <tr><td>C</td><td>2.8541510</td><td>1.3962970</td><td>0.3502350</td></tr> <tr><td>C</td><td>4.9492610</td><td>0.1814300</td><td>0.4488160</td></tr> <tr><td>C</td><td>3.5333000</td><td>2.5801150</td><td>0.6321540</td></tr> <tr><td>H</td><td>1.7788790</td><td>1.4062860</td><td>0.2188160</td></tr> <tr><td>C</td><td>5.6244800</td><td>1.3665670</td><td>0.7266160</td></tr> <tr><td>H</td><td>5.4784480</td><td>-0.7628980</td><td>0.3783460</td></tr> <tr><td>C</td><td>4.9175380</td><td>2.5683250</td><td>0.8179570</td></tr> <tr><td>H</td><td>2.9808900</td><td>3.5124320</td><td>0.7094330</td></tr> <tr><td>H</td><td>6.7008050</td><td>1.3541330</td><td>0.8735280</td></tr> <tr><td>H</td><td>5.4438770</td><td>3.4936590</td><td>1.0365240</td></tr> </tbody> </table>	C	-0.6844280	-1.6240670	-0.4900170	C	0.6847250	-2.0011690	-0.5865080	C	-0.9967730	-0.2326310	-0.2898980	O	3.4920240	-2.1828420	-0.0086960	C	2.9088790	-1.1211150	-0.0342060	O	1.5846530	-0.9643420	-0.3365220	N	-2.1776940	0.3529610	-0.0406570	C	-3.3178950	-0.1887890	0.5120560	C	-3.2776900	-1.2071810	1.5082090	O	-2.2903550	-1.7855790	1.9555810	O	-4.5422950	-1.5008030	1.9710220	H	-0.1937180	0.4723960	-0.4432110	H	-4.2322240	0.3532570	0.3252490	H	-4.3945660	-2.1730550	2.6597160	C	1.0639260	-3.2904650	-0.9502620	C	-1.6470360	-2.6261690	-0.7361410	C	-1.2736260	-3.9093520	-1.1146140	H	-2.0389020	-4.6540490	-1.3135080	C	0.0765920	-4.2426650	-1.2143140	H	0.3754300	-5.2508730	-1.4868890	H	2.1099320	-3.5475580	-1.0096190	H	-2.6970880	-2.3726610	-0.6684620	C	-2.2577030	1.7663330	-0.3705570	C	-2.7487840	2.6677110	0.5764920	C	-1.8490550	2.2051510	-1.6314900	C	-2.8188160	4.0227170	0.2572200	H	-3.0543180	2.3019890	1.5511730	C	-1.9248580	3.5634700	-1.9422910	H	-1.4984070	1.4838220	-2.3629170	C	-2.4082200	4.4729900	-1.0003830	H	-3.1885340	4.7284490	0.9955360	H	-1.6173760	3.9062280	-2.9260630	H	-2.4689640	5.5294710	-1.2459370	C	3.5599440	0.1886270	0.2545600	C	2.8541510	1.3962970	0.3502350	C	4.9492610	0.1814300	0.4488160	C	3.5333000	2.5801150	0.6321540	H	1.7788790	1.4062860	0.2188160	C	5.6244800	1.3665670	0.7266160	H	5.4784480	-0.7628980	0.3783460	C	4.9175380	2.5683250	0.8179570	H	2.9808900	3.5124320	0.7094330	H	6.7008050	1.3541330	0.8735280	H	5.4438770	3.4936590	1.0365240	<p>H (298K) = -1203.833288, G (298K) = -1203.909772 au.</p> <p>Imaginary frequency = 0.</p> <table border="1"> <tbody> <tr><td>C</td><td>-1.3285800</td><td>-1.9625300</td><td>-0.4221780</td></tr> <tr><td>C</td><td>-2.1840370</td><td>-0.8394670</td><td>-0.3987180</td></tr> <tr><td>C</td><td>0.1005520</td><td>-1.9787440</td><td>-0.2331120</td></tr> <tr><td>O</td><td>-0.4279780</td><td>0.5085510</td><td>-2.0137580</td></tr> <tr><td>C</td><td>-0.8608210</td><td>1.0535090</td><td>-1.0210090</td></tr> <tr><td>O</td><td>-1.7275720</td><td>0.4512660</td><td>-0.1473640</td></tr> <tr><td>N</td><td>0.9057210</td><td>-1.1618140</td><td>0.4626700</td></tr> <tr><td>C</td><td>0.6065980</td><td>-0.2832310</td><td>1.4734940</td></tr> <tr><td>C</td><td>-0.5133830</td><td>-0.4431820</td><td>2.3406080</td></tr> <tr><td>O</td><td>-1.3352110</td><td>-1.3553460</td><td>2.3582180</td></tr> <tr><td>O</td><td>-0.5844580</td><td>0.5857820</td><td>3.2589030</td></tr> <tr><td>H</td><td>0.6342310</td><td>-2.7816600</td><td>-0.7273930</td></tr> <tr><td>H</td><td>1.3440360</td><td>0.4798920</td><td>1.6675710</td></tr> <tr><td>H</td><td>-1.3381100</td><td>0.3429720</td><td>3.8261080</td></tr> <tr><td>C</td><td>-3.5544890</td><td>-0.9595780</td><td>-0.6107550</td></tr> <tr><td>C</td><td>-1.9302690</td><td>-3.2007910</td><td>-0.7520670</td></tr> <tr><td>C</td><td>-3.2927140</td><td>-3.3263760</td><td>-0.9748900</td></tr> <tr><td>H</td><td>-3.7143020</td><td>-4.2999050</td><td>-1.2078210</td></tr> <tr><td>C</td><td>-4.1184020</td><td>-2.2001790</td><td>-0.8907720</td></tr> <tr><td>H</td><td>-5.1879190</td><td>-2.2844170</td><td>-1.0593590</td></tr> <tr><td>H</td><td>-4.1597260</td><td>-0.0595820</td><td>-0.5682160</td></tr> <tr><td>H</td><td>-1.2939740</td><td>-4.0806190</td><td>-0.8030780</td></tr> <tr><td>C</td><td>2.3124480</td><td>-1.2289130</td><td>0.0990350</td></tr> <tr><td>C</td><td>3.2681650</td><td>-1.4822720</td><td>1.0839260</td></tr> <tr><td>C</td><td>2.6776650</td><td>-1.0327140</td><td>-1.2335600</td></tr> <tr><td>C</td><td>4.6123650</td><td>-1.5568260</td><td>0.7213850</td></tr> <tr><td>H</td><td>2.9507520</td><td>-1.6317260</td><td>2.1108710</td></tr> <tr><td>C</td><td>4.0269480</td><td>-1.1060740</td><td>-1.5833530</td></tr> <tr><td>H</td><td>1.9118790</td><td>-0.7935810</td><td>-1.9647740</td></tr> <tr><td>C</td><td>4.9926000</td><td>-1.3704100</td><td>-0.6104580</td></tr> <tr><td>H</td><td>5.3618270</td><td>-1.7675980</td><td>1.4788710</td></tr> <tr><td>H</td><td>4.3221880</td><td>-0.9442770</td><td>-2.6161040</td></tr> <tr><td>H</td><td>6.0416250</td><td>-1.4265110</td><td>-0.8876330</td></tr> <tr><td>C</td><td>-0.5555240</td><td>2.4537870</td><td>-0.6198000</td></tr> <tr><td>C</td><td>-0.9478670</td><td>2.9936200</td><td>0.6138230</td></tr> <tr><td>C</td><td>0.1498860</td><td>3.2469680</td><td>-1.5363340</td></tr> <tr><td>C</td><td>-0.6348800</td><td>4.3168970</td><td>0.9196880</td></tr> <tr><td>H</td><td>-1.4665550</td><td>2.3733090</td><td>1.3346730</td></tr> <tr><td>C</td><td>0.4537050</td><td>4.5700690</td><td>-1.2275440</td></tr> <tr><td>H</td><td>0.4461550</td><td>2.8094270</td><td>-2.4839960</td></tr> <tr><td>C</td><td>0.0608550</td><td>5.1068930</td><td>0.0013170</td></tr> <tr><td>H</td><td>-0.9310860</td><td>4.7306740</td><td>1.8795370</td></tr> <tr><td>H</td><td>0.9960830</td><td>5.1825110</td><td>-1.9425620</td></tr> <tr><td>H</td><td>0.2996760</td><td>6.1390390</td><td>0.2442740</td></tr> </tbody> </table>	C	-1.3285800	-1.9625300	-0.4221780	C	-2.1840370	-0.8394670	-0.3987180	C	0.1005520	-1.9787440	-0.2331120	O	-0.4279780	0.5085510	-2.0137580	C	-0.8608210	1.0535090	-1.0210090	O	-1.7275720	0.4512660	-0.1473640	N	0.9057210	-1.1618140	0.4626700	C	0.6065980	-0.2832310	1.4734940	C	-0.5133830	-0.4431820	2.3406080	O	-1.3352110	-1.3553460	2.3582180	O	-0.5844580	0.5857820	3.2589030	H	0.6342310	-2.7816600	-0.7273930	H	1.3440360	0.4798920	1.6675710	H	-1.3381100	0.3429720	3.8261080	C	-3.5544890	-0.9595780	-0.6107550	C	-1.9302690	-3.2007910	-0.7520670	C	-3.2927140	-3.3263760	-0.9748900	H	-3.7143020	-4.2999050	-1.2078210	C	-4.1184020	-2.2001790	-0.8907720	H	-5.1879190	-2.2844170	-1.0593590	H	-4.1597260	-0.0595820	-0.5682160	H	-1.2939740	-4.0806190	-0.8030780	C	2.3124480	-1.2289130	0.0990350	C	3.2681650	-1.4822720	1.0839260	C	2.6776650	-1.0327140	-1.2335600	C	4.6123650	-1.5568260	0.7213850	H	2.9507520	-1.6317260	2.1108710	C	4.0269480	-1.1060740	-1.5833530	H	1.9118790	-0.7935810	-1.9647740	C	4.9926000	-1.3704100	-0.6104580	H	5.3618270	-1.7675980	1.4788710	H	4.3221880	-0.9442770	-2.6161040	H	6.0416250	-1.4265110	-0.8876330	C	-0.5555240	2.4537870	-0.6198000	C	-0.9478670	2.9936200	0.6138230	C	0.1498860	3.2469680	-1.5363340	C	-0.6348800	4.3168970	0.9196880	H	-1.4665550	2.3733090	1.3346730	C	0.4537050	4.5700690	-1.2275440	H	0.4461550	2.8094270	-2.4839960	C	0.0608550	5.1068930	0.0013170	H	-0.9310860	4.7306740	1.8795370	H	0.9960830	5.1825110	-1.9425620	H	0.2996760	6.1390390	0.2442740
C	-0.6844280	-1.6240670	-0.4900170																																																																																																																																																																																																																																																																																																																																																														
C	0.6847250	-2.0011690	-0.5865080																																																																																																																																																																																																																																																																																																																																																														
C	-0.9967730	-0.2326310	-0.2898980																																																																																																																																																																																																																																																																																																																																																														
O	3.4920240	-2.1828420	-0.0086960																																																																																																																																																																																																																																																																																																																																																														
C	2.9088790	-1.1211150	-0.0342060																																																																																																																																																																																																																																																																																																																																																														
O	1.5846530	-0.9643420	-0.3365220																																																																																																																																																																																																																																																																																																																																																														
N	-2.1776940	0.3529610	-0.0406570																																																																																																																																																																																																																																																																																																																																																														
C	-3.3178950	-0.1887890	0.5120560																																																																																																																																																																																																																																																																																																																																																														
C	-3.2776900	-1.2071810	1.5082090																																																																																																																																																																																																																																																																																																																																																														
O	-2.2903550	-1.7855790	1.9555810																																																																																																																																																																																																																																																																																																																																																														
O	-4.5422950	-1.5008030	1.9710220																																																																																																																																																																																																																																																																																																																																																														
H	-0.1937180	0.4723960	-0.4432110																																																																																																																																																																																																																																																																																																																																																														
H	-4.2322240	0.3532570	0.3252490																																																																																																																																																																																																																																																																																																																																																														
H	-4.3945660	-2.1730550	2.6597160																																																																																																																																																																																																																																																																																																																																																														
C	1.0639260	-3.2904650	-0.9502620																																																																																																																																																																																																																																																																																																																																																														
C	-1.6470360	-2.6261690	-0.7361410																																																																																																																																																																																																																																																																																																																																																														
C	-1.2736260	-3.9093520	-1.1146140																																																																																																																																																																																																																																																																																																																																																														
H	-2.0389020	-4.6540490	-1.3135080																																																																																																																																																																																																																																																																																																																																																														
C	0.0765920	-4.2426650	-1.2143140																																																																																																																																																																																																																																																																																																																																																														
H	0.3754300	-5.2508730	-1.4868890																																																																																																																																																																																																																																																																																																																																																														
H	2.1099320	-3.5475580	-1.0096190																																																																																																																																																																																																																																																																																																																																																														
H	-2.6970880	-2.3726610	-0.6684620																																																																																																																																																																																																																																																																																																																																																														
C	-2.2577030	1.7663330	-0.3705570																																																																																																																																																																																																																																																																																																																																																														
C	-2.7487840	2.6677110	0.5764920																																																																																																																																																																																																																																																																																																																																																														
C	-1.8490550	2.2051510	-1.6314900																																																																																																																																																																																																																																																																																																																																																														
C	-2.8188160	4.0227170	0.2572200																																																																																																																																																																																																																																																																																																																																																														
H	-3.0543180	2.3019890	1.5511730																																																																																																																																																																																																																																																																																																																																																														
C	-1.9248580	3.5634700	-1.9422910																																																																																																																																																																																																																																																																																																																																																														
H	-1.4984070	1.4838220	-2.3629170																																																																																																																																																																																																																																																																																																																																																														
C	-2.4082200	4.4729900	-1.0003830																																																																																																																																																																																																																																																																																																																																																														
H	-3.1885340	4.7284490	0.9955360																																																																																																																																																																																																																																																																																																																																																														
H	-1.6173760	3.9062280	-2.9260630																																																																																																																																																																																																																																																																																																																																																														
H	-2.4689640	5.5294710	-1.2459370																																																																																																																																																																																																																																																																																																																																																														
C	3.5599440	0.1886270	0.2545600																																																																																																																																																																																																																																																																																																																																																														
C	2.8541510	1.3962970	0.3502350																																																																																																																																																																																																																																																																																																																																																														
C	4.9492610	0.1814300	0.4488160																																																																																																																																																																																																																																																																																																																																																														
C	3.5333000	2.5801150	0.6321540																																																																																																																																																																																																																																																																																																																																																														
H	1.7788790	1.4062860	0.2188160																																																																																																																																																																																																																																																																																																																																																														
C	5.6244800	1.3665670	0.7266160																																																																																																																																																																																																																																																																																																																																																														
H	5.4784480	-0.7628980	0.3783460																																																																																																																																																																																																																																																																																																																																																														
C	4.9175380	2.5683250	0.8179570																																																																																																																																																																																																																																																																																																																																																														
H	2.9808900	3.5124320	0.7094330																																																																																																																																																																																																																																																																																																																																																														
H	6.7008050	1.3541330	0.8735280																																																																																																																																																																																																																																																																																																																																																														
H	5.4438770	3.4936590	1.0365240																																																																																																																																																																																																																																																																																																																																																														
C	-1.3285800	-1.9625300	-0.4221780																																																																																																																																																																																																																																																																																																																																																														
C	-2.1840370	-0.8394670	-0.3987180																																																																																																																																																																																																																																																																																																																																																														
C	0.1005520	-1.9787440	-0.2331120																																																																																																																																																																																																																																																																																																																																																														
O	-0.4279780	0.5085510	-2.0137580																																																																																																																																																																																																																																																																																																																																																														
C	-0.8608210	1.0535090	-1.0210090																																																																																																																																																																																																																																																																																																																																																														
O	-1.7275720	0.4512660	-0.1473640																																																																																																																																																																																																																																																																																																																																																														
N	0.9057210	-1.1618140	0.4626700																																																																																																																																																																																																																																																																																																																																																														
C	0.6065980	-0.2832310	1.4734940																																																																																																																																																																																																																																																																																																																																																														
C	-0.5133830	-0.4431820	2.3406080																																																																																																																																																																																																																																																																																																																																																														
O	-1.3352110	-1.3553460	2.3582180																																																																																																																																																																																																																																																																																																																																																														
O	-0.5844580	0.5857820	3.2589030																																																																																																																																																																																																																																																																																																																																																														
H	0.6342310	-2.7816600	-0.7273930																																																																																																																																																																																																																																																																																																																																																														
H	1.3440360	0.4798920	1.6675710																																																																																																																																																																																																																																																																																																																																																														
H	-1.3381100	0.3429720	3.8261080																																																																																																																																																																																																																																																																																																																																																														
C	-3.5544890	-0.9595780	-0.6107550																																																																																																																																																																																																																																																																																																																																																														
C	-1.9302690	-3.2007910	-0.7520670																																																																																																																																																																																																																																																																																																																																																														
C	-3.2927140	-3.3263760	-0.9748900																																																																																																																																																																																																																																																																																																																																																														
H	-3.7143020	-4.2999050	-1.2078210																																																																																																																																																																																																																																																																																																																																																														
C	-4.1184020	-2.2001790	-0.8907720																																																																																																																																																																																																																																																																																																																																																														
H	-5.1879190	-2.2844170	-1.0593590																																																																																																																																																																																																																																																																																																																																																														
H	-4.1597260	-0.0595820	-0.5682160																																																																																																																																																																																																																																																																																																																																																														
H	-1.2939740	-4.0806190	-0.8030780																																																																																																																																																																																																																																																																																																																																																														
C	2.3124480	-1.2289130	0.0990350																																																																																																																																																																																																																																																																																																																																																														
C	3.2681650	-1.4822720	1.0839260																																																																																																																																																																																																																																																																																																																																																														
C	2.6776650	-1.0327140	-1.2335600																																																																																																																																																																																																																																																																																																																																																														
C	4.6123650	-1.5568260	0.7213850																																																																																																																																																																																																																																																																																																																																																														
H	2.9507520	-1.6317260	2.1108710																																																																																																																																																																																																																																																																																																																																																														
C	4.0269480	-1.1060740	-1.5833530																																																																																																																																																																																																																																																																																																																																																														
H	1.9118790	-0.7935810	-1.9647740																																																																																																																																																																																																																																																																																																																																																														
C	4.9926000	-1.3704100	-0.6104580																																																																																																																																																																																																																																																																																																																																																														
H	5.3618270	-1.7675980	1.4788710																																																																																																																																																																																																																																																																																																																																																														
H	4.3221880	-0.9442770	-2.6161040																																																																																																																																																																																																																																																																																																																																																														
H	6.0416250	-1.4265110	-0.8876330																																																																																																																																																																																																																																																																																																																																																														
C	-0.5555240	2.4537870	-0.6198000																																																																																																																																																																																																																																																																																																																																																														
C	-0.9478670	2.9936200	0.6138230																																																																																																																																																																																																																																																																																																																																																														
C	0.1498860	3.2469680	-1.5363340																																																																																																																																																																																																																																																																																																																																																														
C	-0.6348800	4.3168970	0.9196880																																																																																																																																																																																																																																																																																																																																																														
H	-1.4665550	2.3733090	1.3346730																																																																																																																																																																																																																																																																																																																																																														
C	0.4537050	4.5700690	-1.2275440																																																																																																																																																																																																																																																																																																																																																														
H	0.4461550	2.8094270	-2.4839960																																																																																																																																																																																																																																																																																																																																																														
C	0.0608550	5.1068930	0.0013170																																																																																																																																																																																																																																																																																																																																																														
H	-0.9310860	4.7306740	1.8795370																																																																																																																																																																																																																																																																																																																																																														
H	0.9960830	5.1825110	-1.9425620																																																																																																																																																																																																																																																																																																																																																														
H	0.2996760	6.1390390	0.2442740																																																																																																																																																																																																																																																																																																																																																														
<p>TS Ylide U-3' (X=Y=H) → Ylide U-3 (X=Y=H) (TS_{U-3'/U-3})</p>  <p>E = -1204.18310772, H (0K) = -1203.842027,</p>	<p>TS Ylide S-3' (X=Y=H) → Ylide S-3'' (X=Y=H) (TS_{S-3'/S-3''})</p>  <p>E = -1204.19575301, H (0K) = -1203.853692,</p>																																																																																																																																																																																																																																																																																																																																																																

H (298K) = -1203.818970, G (298K) = -1203.897292 au.				H (298K) = -1203.831014, G (298K) = -1203.907243 au.			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-0.5284960	2.0777790	-0.6351510	C	0.2888170	1.9221640	0.2568790
C	0.8616440	2.0375900	-0.4608050	C	-1.1175000	2.1441250	0.2898630
C	-1.3211510	0.8343770	-0.7425290	C	0.7685780	0.5580860	0.2316480
O	2.9865510	0.8390370	-1.7857650	O	-3.9169740	1.8999310	-0.3015240
C	2.4714070	0.2927670	-0.8356780	C	-3.2119950	0.9304180	-0.1252310
O	1.4052440	0.7963130	-0.1445630	O	-1.8799680	0.9815570	0.1863950
N	-1.8777150	0.0909530	0.2111450	N	1.9892870	0.1135060	-0.1020680
C	-1.9204070	0.1304060	1.5805410	C	2.9411170	0.8163630	-0.7889960
C	-1.1607030	0.9720120	2.4512180	C	4.3402980	0.5109990	-0.7341230
O	-0.2730370	1.7769800	2.1926650	O	4.9186880	-0.3506280	-0.0808160
O	-1.5410150	0.7504750	3.7581510	O	5.0433270	1.3690180	-1.5503760
H	-1.4879220	0.4429180	-1.7394930	H	0.0756990	-0.2213920	0.5059890
H	-2.6094680	-0.5708410	2.0227090	H	2.6054790	1.6963780	-1.3143580
H	-0.9641320	1.3393250	4.2763880	H	5.9729390	1.1037690	-1.4331580
C	1.6397280	3.1881370	-0.5099630	C	-1.6542530	3.4192840	0.4552680
C	-1.1253280	3.3211320	-0.8774750	C	-0.7952500	4.5131250	0.5783030
C	-0.3603200	4.4868200	-0.9235290	H	-1.2178210	5.5067950	0.6952380
H	-0.8418780	5.4438690	-1.1026780	C	0.5873650	4.3321960	0.5435940
C	1.0207410	4.4166820	-0.7425020	C	1.1192320	3.0597220	0.3757230
H	1.6241220	5.3193090	-0.7812460	H	1.2553920	5.1827320	0.6441650
H	2.7115850	3.1213340	-0.3670700	H	2.1948970	2.9316520	0.3671180
H	-2.2004890	3.3673820	-1.0275800	H	-2.7246630	3.5532790	0.4703410
C	-2.6395750	-1.0428940	-0.3206660	C	2.2338740	-1.2885630	0.2185580
C	-3.8953200	-0.8191710	-0.8778740	C	2.0842250	-1.7219350	1.5336400
C	-2.0855720	-2.3192250	-0.2542590	C	2.5506860	-2.1793430	-0.8060390
C	-4.6141520	-1.9047630	-1.3832010	C	2.2604460	-3.0748320	1.8285580
H	-4.3002380	0.1875290	-0.9067060	H	1.8566370	-1.0033400	2.3144360
C	-2.8095460	-3.3957180	-0.7681790	C	2.7191040	-3.5275790	-0.5026320
H	-1.1021190	-2.4561020	0.1842170	H	2.6607940	-1.8106040	-1.8204370
C	-4.0721950	-3.1899950	-1.3299290	C	2.5762000	-3.9776500	0.8132400
H	-5.5973470	-1.7431080	-1.8154360	H	2.1582440	-3.4178020	2.8540990
H	-2.3843610	-4.3944360	-0.7310030	H	2.9621370	-4.2288800	-1.2956910
H	-4.6330850	-4.0318610	-1.7257300	H	2.7147420	-5.0299350	1.0451260
C	2.8965260	-1.0183770	-0.2706650	C	-3.6945450	-0.4760760	-0.2166960
C	2.3249200	-1.5540450	0.8933120	C	-2.8447740	-1.5887100	-0.1373300
C	3.9094070	-1.7194840	-0.9389350	C	-5.0716770	-0.6676290	-0.4045970
C	2.7662650	-2.7848980	1.3769880	C	-3.3700570	-2.8752840	-0.2408520
H	1.5520280	-0.9990840	1.4136940	H	-1.7784190	-1.4476090	-0.0086720
C	4.3438010	-2.9500790	-0.4529980	C	-5.5926210	-1.9545610	-0.5039540
H	4.3411890	-1.2828570	-1.8336080	H	-5.7137920	0.2042800	-0.4697060
C	3.7723680	-3.4841060	0.7051850	C	-4.7425970	-3.0605660	-0.4215710
H	2.3283970	-3.1967240	2.2821820	H	-2.7068410	-3.7336590	-0.1819750
H	5.1281080	-3.4921620	-0.9740280	H	-6.6601790	-2.0963680	-0.6465550
H	4.1134190	-4.4432860	1.0860480	H	-5.1488710	-4.0654010	-0.5004260
TS Ylide U-3 (X=Y=H) → <i>endo</i>-2-adduct (X=Y=H) (TS _{U-3/endo-2})				TS Ylide S-3'' (X=Y=H) → Ylide U-3' (X=Y=H) (TS _{S-3''/U-3'})			
							

E = -1204.17894925, H (0K) = -1203.836460, H (298K) = -1203.814707, G (298K) = -1203.886945 au.				E = -1204.17062946, H (0K) = -1203.830251, H (298K) = -1203.806929, G (298K) = -1203.885871 au.			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	2.4780540	4.1101210	-0.5335830	C	-0.6019550	1.8082990	-0.1681130
C	1.2023390	4.5851110	-0.8740420	C	0.7594770	2.1437600	0.0538520
C	0.1409130	3.6971070	-0.9009780	C	-0.9249810	0.3964180	-0.2260880
C	0.3041610	2.3349140	-0.5608460	O	3.1606880	1.7928250	-1.2595770
C	1.6112010	1.8584110	-0.2680620	C	2.8511340	1.0267630	-0.3789300
C	2.6820410	2.7676380	-0.2515320	O	1.6457850	1.1038160	0.3004580
C	-0.8973690	1.5271750	-0.5775420	N	-2.0736390	-0.2093910	-0.3480200
O	0.2677640	-0.1217870	-1.5809480	C	-3.3529930	0.4604070	-0.4641950
C	0.8293270	-0.4377940	-0.4698730	C	-4.1835700	0.4805340	0.6614740
O	1.8951910	0.5759630	-0.0231310	O	-3.9199090	0.1119820	1.8218900
N	-1.2961410	0.5562080	0.2475810	O	-5.4292510	1.0307830	0.3967190
C	-0.2778490	-0.3222170	0.7905250	H	-0.0719490	-0.2703890	-0.1533720
C	0.2822850	0.1921250	2.0947390	H	-3.7071390	0.5813860	-1.4796750
O	0.1724670	1.3206720	2.5203840	H	-5.8690270	0.9995240	1.2640890
O	0.9280480	-0.7899890	2.7670430	C	1.1799810	3.4672220	0.1168800
H	3.3227600	4.7936900	-0.5115800	C	0.2433430	4.4874860	-0.0416270
H	1.0488410	5.6316390	-1.1175770	H	0.5728640	5.5216690	0.0067690
H	-0.8534380	4.0504460	-1.1643960	C	-1.1053820	4.1883870	-0.2544490
H	3.6705290	2.3794510	-0.0286050	C	-1.5262090	2.8671990	-0.3173760
H	-1.7179080	1.9537410	-1.1500680	H	-1.8300830	4.9882400	-0.3708300
H	-0.7145860	-1.3086480	0.9474550	H	-2.5657020	2.5986660	-0.4702720
H	1.2904750	-0.3701250	3.5699030	H	2.2252390	3.6922210	0.2870160
C	-2.6172180	0.0016600	0.0567900	C	-2.0448070	-1.6650650	-0.4399590
C	-3.4944040	-0.0247480	1.1424990	C	-1.3052460	-2.2729320	-1.4577590
C	-2.9922180	-0.5119620	-1.1874140	C	-2.7842070	-2.4249900	0.4723530
C	-4.7696410	-0.5653470	0.9762010	C	-1.3004830	-3.6656040	-1.5634670
H	-3.1774180	0.3868460	2.0961320	H	-0.7639890	-1.6630800	-2.1761240
C	-4.2737650	-1.0421780	-1.3438790	C	-2.7604130	-3.8128300	0.3578680
H	-2.2678640	-0.5127450	-1.9958630	H	-3.3393510	-1.9114040	1.2516470
C	-5.1614600	-1.0697600	-0.2662140	C	-2.0240310	-4.4370250	-0.6551690
H	-5.4590800	-0.5843290	1.8154380	H	-0.7362690	-4.1406540	-2.3612130
H	-4.5730720	-1.4448880	-2.3074660	H	-3.3209210	-4.4128890	1.0693750
H	-6.1563730	-1.4874510	-0.3925460	H	-2.0194450	-5.5204080	-0.7368530
C	1.5317380	-1.7925840	-0.4299070	C	3.6706020	-0.1103560	0.1075210
C	2.6263610	-2.0631210	0.3977410	C	3.2875090	-0.9138890	1.1921800
C	1.0410910	-2.8011760	-1.2671160	C	4.8783800	-0.3651950	-0.5598360
C	3.2164190	-3.3282890	0.3893480	C	4.1080620	-1.9638100	1.5994610
H	3.0206930	-1.2833260	1.0372310	H	2.3587170	-0.7126240	1.7137640
C	1.6264510	-4.0667630	-1.2678420	C	5.6922180	-1.4168500	-0.1497760
H	0.2109100	-2.5721490	-1.9268900	H	5.1585800	0.2700900	-1.3935320
C	2.7171130	-4.3348980	-0.4382640	C	5.3076410	-2.2170560	0.9298470
H	4.0716480	-3.5253090	1.0310080	H	3.8113780	-2.5842460	2.4401230
H	1.2372150	-4.8405340	-1.9248810	H	6.6257500	-1.6132530	-0.6691410
H	3.1784690	-5.3191820	-0.4416310	H	5.9438920	-3.0375970	1.2503030
Ylide S-3" (X=Y=H) 				endo-2-adduct (X=CN, Y=H) 			

<p>E = -1204.19794783, H (0K) = -1203.855921, H (298K) = -1203.832360, G (298K) = -1203.912177 au.</p> <p>Imaginary frequency = 0.</p> <table border="1"> <tbody> <tr><td>C</td><td>0.3790010</td><td>1.9039310</td><td>0.0010860</td></tr> <tr><td>C</td><td>-1.0117650</td><td>2.1675210</td><td>-0.0992140</td></tr> <tr><td>C</td><td>0.8023040</td><td>0.5229350</td><td>0.0250370</td></tr> <tr><td>O</td><td>-3.3059990</td><td>1.5591400</td><td>1.3264030</td></tr> <tr><td>C</td><td>-2.9705880</td><td>0.8558100</td><td>0.4015610</td></tr> <tr><td>O</td><td>-1.8377170</td><td>1.0714490</td><td>-0.3499780</td></tr> <tr><td>N</td><td>2.0391800</td><td>0.0274200</td><td>-0.1330670</td></tr> <tr><td>C</td><td>3.1089060</td><td>0.6940840</td><td>-0.6648470</td></tr> <tr><td>C</td><td>4.4721740</td><td>0.3385520</td><td>-0.3998850</td></tr> <tr><td>O</td><td>4.9135760</td><td>-0.5397910</td><td>0.3326420</td></tr> <tr><td>O</td><td>5.3207190</td><td>1.1670610</td><td>-1.1004280</td></tr> <tr><td>H</td><td>0.0403230</td><td>-0.2287010</td><td>0.1654020</td></tr> <tr><td>H</td><td>2.8897430</td><td>1.5811150</td><td>-1.2373220</td></tr> <tr><td>H</td><td>6.2119350</td><td>0.8700260</td><td>-0.8438630</td></tr> <tr><td>C</td><td>-1.5313040</td><td>3.4545090</td><td>-0.0388580</td></tr> <tr><td>C</td><td>-0.6700750</td><td>4.5358590</td><td>0.1437350</td></tr> <tr><td>H</td><td>-1.0729560</td><td>5.5432960</td><td>0.1867700</td></tr> <tr><td>C</td><td>0.7042070</td><td>4.3148870</td><td>0.2609440</td></tr> <tr><td>C</td><td>1.2218950</td><td>3.0283890</td><td>0.1754520</td></tr> <tr><td>H</td><td>1.3805450</td><td>5.1516930</td><td>0.4099470</td></tr> <tr><td>H</td><td>2.2902390</td><td>2.8819640</td><td>0.2742150</td></tr> <tr><td>H</td><td>-2.6001240</td><td>3.6039120</td><td>-0.1296420</td></tr> <tr><td>C</td><td>2.1778660</td><td>-1.3851780</td><td>0.2027130</td></tr> <tr><td>C</td><td>1.8075460</td><td>-1.8233210</td><td>1.4718670</td></tr> <tr><td>C</td><td>2.6199480</td><td>-2.2790830</td><td>-0.7716740</td></tr> <tr><td>C</td><td>1.8875330</td><td>-3.1839920</td><td>1.7720570</td></tr> <tr><td>H</td><td>1.4843980</td><td>-1.1033890</td><td>2.2169170</td></tr> <tr><td>C</td><td>2.6910370</td><td>-3.6347720</td><td>-0.4642280</td></tr> <tr><td>H</td><td>2.9002670</td><td>-1.9069020</td><td>-1.7514840</td></tr> <tr><td>C</td><td>2.3273050</td><td>-4.0896740</td><td>0.8067170</td></tr> <tr><td>H</td><td>1.6121000</td><td>-3.5312040</td><td>2.7636730</td></tr> <tr><td>H</td><td>3.0302390</td><td>-4.3384550</td><td>-1.2189770</td></tr> <tr><td>H</td><td>2.3896270</td><td>-5.1482630</td><td>1.0428010</td></tr> <tr><td>C</td><td>-3.7083260</td><td>-0.3473870</td><td>-0.0674270</td></tr> <tr><td>C</td><td>-3.2959200</td><td>-1.1090700</td><td>-1.1707350</td></tr> <tr><td>C</td><td>-4.8636930</td><td>-0.7117990</td><td>0.6393470</td></tr> <tr><td>C</td><td>-4.0353600</td><td>-2.2251340</td><td>-1.5580850</td></tr> <tr><td>H</td><td>-2.4048540</td><td>-0.8235930</td><td>-1.7181120</td></tr> <tr><td>C</td><td>-5.5979170</td><td>-1.8279170</td><td>0.2487500</td></tr> <tr><td>H</td><td>-5.1669030</td><td>-0.1083310</td><td>1.4884990</td></tr> <tr><td>C</td><td>-5.1845190</td><td>-2.5857660</td><td>-0.8503890</td></tr> <tr><td>H</td><td>-3.7150080</td><td>-2.8136880</td><td>-2.4131610</td></tr> <tr><td>H</td><td>-6.4918720</td><td>-2.1077580</td><td>0.7988990</td></tr> <tr><td>H</td><td>-5.7581340</td><td>-3.4568450</td><td>-1.1557400</td></tr> </tbody> </table>	C	0.3790010	1.9039310	0.0010860	C	-1.0117650	2.1675210	-0.0992140	C	0.8023040	0.5229350	0.0250370	O	-3.3059990	1.5591400	1.3264030	C	-2.9705880	0.8558100	0.4015610	O	-1.8377170	1.0714490	-0.3499780	N	2.0391800	0.0274200	-0.1330670	C	3.1089060	0.6940840	-0.6648470	C	4.4721740	0.3385520	-0.3998850	O	4.9135760	-0.5397910	0.3326420	O	5.3207190	1.1670610	-1.1004280	H	0.0403230	-0.2287010	0.1654020	H	2.8897430	1.5811150	-1.2373220	H	6.2119350	0.8700260	-0.8438630	C	-1.5313040	3.4545090	-0.0388580	C	-0.6700750	4.5358590	0.1437350	H	-1.0729560	5.5432960	0.1867700	C	0.7042070	4.3148870	0.2609440	C	1.2218950	3.0283890	0.1754520	H	1.3805450	5.1516930	0.4099470	H	2.2902390	2.8819640	0.2742150	H	-2.6001240	3.6039120	-0.1296420	C	2.1778660	-1.3851780	0.2027130	C	1.8075460	-1.8233210	1.4718670	C	2.6199480	-2.2790830	-0.7716740	C	1.8875330	-3.1839920	1.7720570	H	1.4843980	-1.1033890	2.2169170	C	2.6910370	-3.6347720	-0.4642280	H	2.9002670	-1.9069020	-1.7514840	C	2.3273050	-4.0896740	0.8067170	H	1.6121000	-3.5312040	2.7636730	H	3.0302390	-4.3384550	-1.2189770	H	2.3896270	-5.1482630	1.0428010	C	-3.7083260	-0.3473870	-0.0674270	C	-3.2959200	-1.1090700	-1.1707350	C	-4.8636930	-0.7117990	0.6393470	C	-4.0353600	-2.2251340	-1.5580850	H	-2.4048540	-0.8235930	-1.7181120	C	-5.5979170	-1.8279170	0.2487500	H	-5.1669030	-0.1083310	1.4884990	C	-5.1845190	-2.5857660	-0.8503890	H	-3.7150080	-2.8136880	-2.4131610	H	-6.4918720	-2.1077580	0.7988990	H	-5.7581340	-3.4568450	-1.1557400	<p>E = -1296.45709480, H (0K) = -1296.113400, H (298K) = -1296.089943, G (298K) = -1296.167278 au.</p> <p>Imaginary frequency = 0.</p> <table border="1"> <tbody> <tr><td>C</td><td>2.4462230</td><td>-4.3331660</td><td>-0.3932750</td></tr> <tr><td>C</td><td>3.4282860</td><td>-3.5266350</td><td>-0.9746440</td></tr> <tr><td>C</td><td>3.1558660</td><td>-2.1821820</td><td>-1.2295710</td></tr> <tr><td>C</td><td>1.9161980</td><td>-1.6378700</td><td>-0.8987070</td></tr> <tr><td>C</td><td>0.9465440</td><td>-2.4593570</td><td>-0.3110090</td></tr> <tr><td>C</td><td>1.1980030</td><td>-3.8065540</td><td>-0.0621770</td></tr> <tr><td>C</td><td>1.5178890</td><td>-0.2035820</td><td>-1.1613870</td></tr> <tr><td>O</td><td>0.1012860</td><td>-0.2246180</td><td>-1.4860350</td></tr> <tr><td>C</td><td>-0.4763050</td><td>-0.5611270</td><td>-0.2501280</td></tr> <tr><td>O</td><td>-0.2934700</td><td>-1.9553090</td><td>0.0270400</td></tr> <tr><td>N</td><td>1.6017620</td><td>0.6125220</td><td>0.0353800</td></tr> <tr><td>C</td><td>0.3730850</td><td>0.3185730</td><td>0.7766330</td></tr> <tr><td>C</td><td>0.5995990</td><td>-0.3650740</td><td>2.1219440</td></tr> <tr><td>O</td><td>1.6603640</td><td>-0.6977260</td><td>2.5898010</td></tr> <tr><td>O</td><td>-0.5812640</td><td>-0.5156650</td><td>2.7714520</td></tr> <tr><td>H</td><td>2.6503420</td><td>-5.3819650</td><td>-0.1966740</td></tr> <tr><td>H</td><td>4.3966540</td><td>-3.9439840</td><td>-1.2334380</td></tr> <tr><td>H</td><td>3.9097140</td><td>-1.5482450</td><td>-1.6908540</td></tr> <tr><td>H</td><td>0.4212870</td><td>-4.4190380</td><td>0.3846420</td></tr> <tr><td>H</td><td>2.0651780</td><td>0.2334180</td><td>-1.9948800</td></tr> <tr><td>H</td><td>-0.1800980</td><td>1.2425000</td><td>0.9742160</td></tr> <tr><td>H</td><td>-0.3730330</td><td>-0.9516040</td><td>3.6195110</td></tr> <tr><td>C</td><td>1.9877180</td><td>1.9845440</td><td>-0.0543540</td></tr> <tr><td>C</td><td>2.4989180</td><td>2.5890550</td><td>1.1033660</td></tr> <tr><td>C</td><td>1.8735910</td><td>2.7425870</td><td>-1.2289750</td></tr> <tr><td>C</td><td>2.8795520</td><td>3.9296250</td><td>1.0881790</td></tr> <tr><td>H</td><td>2.6136250</td><td>1.9853270</td><td>1.9987040</td></tr> <tr><td>C</td><td>2.2815110</td><td>4.0776320</td><td>-1.2424580</td></tr> <tr><td>H</td><td>1.4473300</td><td>2.3046240</td><td>-2.1267150</td></tr> <tr><td>C</td><td>2.7802540</td><td>4.6788750</td><td>-0.0863470</td></tr> <tr><td>H</td><td>3.2745770</td><td>4.3837500</td><td>1.9930580</td></tr> <tr><td>H</td><td>2.1903490</td><td>4.6529270</td><td>-2.1600630</td></tr> <tr><td>H</td><td>3.0896200</td><td>5.7200520</td><td>-0.1007190</td></tr> <tr><td>C</td><td>-1.9600800</td><td>-0.2725070</td><td>-0.2609930</td></tr> <tr><td>C</td><td>-2.8589160</td><td>-1.0847120</td><td>0.4385330</td></tr> <tr><td>C</td><td>-2.4354490</td><td>0.8416870</td><td>-0.9638120</td></tr> <tr><td>C</td><td>-4.2183010</td><td>-0.7889370</td><td>0.4374320</td></tr> <tr><td>H</td><td>-2.4909450</td><td>-1.9476560</td><td>0.9789850</td></tr> <tr><td>C</td><td>-3.7923130</td><td>1.1439250</td><td>-0.9705000</td></tr> <tr><td>H</td><td>-1.7390150</td><td>1.4627280</td><td>-1.5164640</td></tr> <tr><td>C</td><td>-4.6942430</td><td>0.3283220</td><td>-0.2670750</td></tr> <tr><td>H</td><td>-4.9165630</td><td>-1.4197650</td><td>0.9777760</td></tr> <tr><td>H</td><td>-4.1609490</td><td>2.0039980</td><td>-1.5198860</td></tr> <tr><td>C</td><td>-6.0951790</td><td>0.6351240</td><td>-0.2697850</td></tr> <tr><td>N</td><td>-7.2314890</td><td>0.8846240</td><td>-0.2711790</td></tr> </tbody> </table>	C	2.4462230	-4.3331660	-0.3932750	C	3.4282860	-3.5266350	-0.9746440	C	3.1558660	-2.1821820	-1.2295710	C	1.9161980	-1.6378700	-0.8987070	C	0.9465440	-2.4593570	-0.3110090	C	1.1980030	-3.8065540	-0.0621770	C	1.5178890	-0.2035820	-1.1613870	O	0.1012860	-0.2246180	-1.4860350	C	-0.4763050	-0.5611270	-0.2501280	O	-0.2934700	-1.9553090	0.0270400	N	1.6017620	0.6125220	0.0353800	C	0.3730850	0.3185730	0.7766330	C	0.5995990	-0.3650740	2.1219440	O	1.6603640	-0.6977260	2.5898010	O	-0.5812640	-0.5156650	2.7714520	H	2.6503420	-5.3819650	-0.1966740	H	4.3966540	-3.9439840	-1.2334380	H	3.9097140	-1.5482450	-1.6908540	H	0.4212870	-4.4190380	0.3846420	H	2.0651780	0.2334180	-1.9948800	H	-0.1800980	1.2425000	0.9742160	H	-0.3730330	-0.9516040	3.6195110	C	1.9877180	1.9845440	-0.0543540	C	2.4989180	2.5890550	1.1033660	C	1.8735910	2.7425870	-1.2289750	C	2.8795520	3.9296250	1.0881790	H	2.6136250	1.9853270	1.9987040	C	2.2815110	4.0776320	-1.2424580	H	1.4473300	2.3046240	-2.1267150	C	2.7802540	4.6788750	-0.0863470	H	3.2745770	4.3837500	1.9930580	H	2.1903490	4.6529270	-2.1600630	H	3.0896200	5.7200520	-0.1007190	C	-1.9600800	-0.2725070	-0.2609930	C	-2.8589160	-1.0847120	0.4385330	C	-2.4354490	0.8416870	-0.9638120	C	-4.2183010	-0.7889370	0.4374320	H	-2.4909450	-1.9476560	0.9789850	C	-3.7923130	1.1439250	-0.9705000	H	-1.7390150	1.4627280	-1.5164640	C	-4.6942430	0.3283220	-0.2670750	H	-4.9165630	-1.4197650	0.9777760	H	-4.1609490	2.0039980	-1.5198860	C	-6.0951790	0.6351240	-0.2697850	N	-7.2314890	0.8846240	-0.2711790
C	0.3790010	1.9039310	0.0010860																																																																																																																																																																																																																																																																																																																																																																		
C	-1.0117650	2.1675210	-0.0992140																																																																																																																																																																																																																																																																																																																																																																		
C	0.8023040	0.5229350	0.0250370																																																																																																																																																																																																																																																																																																																																																																		
O	-3.3059990	1.5591400	1.3264030																																																																																																																																																																																																																																																																																																																																																																		
C	-2.9705880	0.8558100	0.4015610																																																																																																																																																																																																																																																																																																																																																																		
O	-1.8377170	1.0714490	-0.3499780																																																																																																																																																																																																																																																																																																																																																																		
N	2.0391800	0.0274200	-0.1330670																																																																																																																																																																																																																																																																																																																																																																		
C	3.1089060	0.6940840	-0.6648470																																																																																																																																																																																																																																																																																																																																																																		
C	4.4721740	0.3385520	-0.3998850																																																																																																																																																																																																																																																																																																																																																																		
O	4.9135760	-0.5397910	0.3326420																																																																																																																																																																																																																																																																																																																																																																		
O	5.3207190	1.1670610	-1.1004280																																																																																																																																																																																																																																																																																																																																																																		
H	0.0403230	-0.2287010	0.1654020																																																																																																																																																																																																																																																																																																																																																																		
H	2.8897430	1.5811150	-1.2373220																																																																																																																																																																																																																																																																																																																																																																		
H	6.2119350	0.8700260	-0.8438630																																																																																																																																																																																																																																																																																																																																																																		
C	-1.5313040	3.4545090	-0.0388580																																																																																																																																																																																																																																																																																																																																																																		
C	-0.6700750	4.5358590	0.1437350																																																																																																																																																																																																																																																																																																																																																																		
H	-1.0729560	5.5432960	0.1867700																																																																																																																																																																																																																																																																																																																																																																		
C	0.7042070	4.3148870	0.2609440																																																																																																																																																																																																																																																																																																																																																																		
C	1.2218950	3.0283890	0.1754520																																																																																																																																																																																																																																																																																																																																																																		
H	1.3805450	5.1516930	0.4099470																																																																																																																																																																																																																																																																																																																																																																		
H	2.2902390	2.8819640	0.2742150																																																																																																																																																																																																																																																																																																																																																																		
H	-2.6001240	3.6039120	-0.1296420																																																																																																																																																																																																																																																																																																																																																																		
C	2.1778660	-1.3851780	0.2027130																																																																																																																																																																																																																																																																																																																																																																		
C	1.8075460	-1.8233210	1.4718670																																																																																																																																																																																																																																																																																																																																																																		
C	2.6199480	-2.2790830	-0.7716740																																																																																																																																																																																																																																																																																																																																																																		
C	1.8875330	-3.1839920	1.7720570																																																																																																																																																																																																																																																																																																																																																																		
H	1.4843980	-1.1033890	2.2169170																																																																																																																																																																																																																																																																																																																																																																		
C	2.6910370	-3.6347720	-0.4642280																																																																																																																																																																																																																																																																																																																																																																		
H	2.9002670	-1.9069020	-1.7514840																																																																																																																																																																																																																																																																																																																																																																		
C	2.3273050	-4.0896740	0.8067170																																																																																																																																																																																																																																																																																																																																																																		
H	1.6121000	-3.5312040	2.7636730																																																																																																																																																																																																																																																																																																																																																																		
H	3.0302390	-4.3384550	-1.2189770																																																																																																																																																																																																																																																																																																																																																																		
H	2.3896270	-5.1482630	1.0428010																																																																																																																																																																																																																																																																																																																																																																		
C	-3.7083260	-0.3473870	-0.0674270																																																																																																																																																																																																																																																																																																																																																																		
C	-3.2959200	-1.1090700	-1.1707350																																																																																																																																																																																																																																																																																																																																																																		
C	-4.8636930	-0.7117990	0.6393470																																																																																																																																																																																																																																																																																																																																																																		
C	-4.0353600	-2.2251340	-1.5580850																																																																																																																																																																																																																																																																																																																																																																		
H	-2.4048540	-0.8235930	-1.7181120																																																																																																																																																																																																																																																																																																																																																																		
C	-5.5979170	-1.8279170	0.2487500																																																																																																																																																																																																																																																																																																																																																																		
H	-5.1669030	-0.1083310	1.4884990																																																																																																																																																																																																																																																																																																																																																																		
C	-5.1845190	-2.5857660	-0.8503890																																																																																																																																																																																																																																																																																																																																																																		
H	-3.7150080	-2.8136880	-2.4131610																																																																																																																																																																																																																																																																																																																																																																		
H	-6.4918720	-2.1077580	0.7988990																																																																																																																																																																																																																																																																																																																																																																		
H	-5.7581340	-3.4568450	-1.1557400																																																																																																																																																																																																																																																																																																																																																																		
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C	3.4282860	-3.5266350	-0.9746440																																																																																																																																																																																																																																																																																																																																																																		
C	3.1558660	-2.1821820	-1.2295710																																																																																																																																																																																																																																																																																																																																																																		
C	1.9161980	-1.6378700	-0.8987070																																																																																																																																																																																																																																																																																																																																																																		
C	0.9465440	-2.4593570	-0.3110090																																																																																																																																																																																																																																																																																																																																																																		
C	1.1980030	-3.8065540	-0.0621770																																																																																																																																																																																																																																																																																																																																																																		
C	1.5178890	-0.2035820	-1.1613870																																																																																																																																																																																																																																																																																																																																																																		
O	0.1012860	-0.2246180	-1.4860350																																																																																																																																																																																																																																																																																																																																																																		
C	-0.4763050	-0.5611270	-0.2501280																																																																																																																																																																																																																																																																																																																																																																		
O	-0.2934700	-1.9553090	0.0270400																																																																																																																																																																																																																																																																																																																																																																		
N	1.6017620	0.6125220	0.0353800																																																																																																																																																																																																																																																																																																																																																																		
C	0.3730850	0.3185730	0.7766330																																																																																																																																																																																																																																																																																																																																																																		
C	0.5995990	-0.3650740	2.1219440																																																																																																																																																																																																																																																																																																																																																																		
O	1.6603640	-0.6977260	2.5898010																																																																																																																																																																																																																																																																																																																																																																		
O	-0.5812640	-0.5156650	2.7714520																																																																																																																																																																																																																																																																																																																																																																		
H	2.6503420	-5.3819650	-0.1966740																																																																																																																																																																																																																																																																																																																																																																		
H	4.3966540	-3.9439840	-1.2334380																																																																																																																																																																																																																																																																																																																																																																		
H	3.9097140	-1.5482450	-1.6908540																																																																																																																																																																																																																																																																																																																																																																		
H	0.4212870	-4.4190380	0.3846420																																																																																																																																																																																																																																																																																																																																																																		
H	2.0651780	0.2334180	-1.9948800																																																																																																																																																																																																																																																																																																																																																																		
H	-0.1800980	1.2425000	0.9742160																																																																																																																																																																																																																																																																																																																																																																		
H	-0.3730330	-0.9516040	3.6195110																																																																																																																																																																																																																																																																																																																																																																		
C	1.9877180	1.9845440	-0.0543540																																																																																																																																																																																																																																																																																																																																																																		
C	2.4989180	2.5890550	1.1033660																																																																																																																																																																																																																																																																																																																																																																		
C	1.8735910	2.7425870	-1.2289750																																																																																																																																																																																																																																																																																																																																																																		
C	2.8795520	3.9296250	1.0881790																																																																																																																																																																																																																																																																																																																																																																		
H	2.6136250	1.9853270	1.9987040																																																																																																																																																																																																																																																																																																																																																																		
C	2.2815110	4.0776320	-1.2424580																																																																																																																																																																																																																																																																																																																																																																		
H	1.4473300	2.3046240	-2.1267150																																																																																																																																																																																																																																																																																																																																																																		
C	2.7802540	4.6788750	-0.0863470																																																																																																																																																																																																																																																																																																																																																																		
H	3.2745770	4.3837500	1.9930580																																																																																																																																																																																																																																																																																																																																																																		
H	2.1903490	4.6529270	-2.1600630																																																																																																																																																																																																																																																																																																																																																																		
H	3.0896200	5.7200520	-0.1007190																																																																																																																																																																																																																																																																																																																																																																		
C	-1.9600800	-0.2725070	-0.2609930																																																																																																																																																																																																																																																																																																																																																																		
C	-2.8589160	-1.0847120	0.4385330																																																																																																																																																																																																																																																																																																																																																																		
C	-2.4354490	0.8416870	-0.9638120																																																																																																																																																																																																																																																																																																																																																																		
C	-4.2183010	-0.7889370	0.4374320																																																																																																																																																																																																																																																																																																																																																																		
H	-2.4909450	-1.9476560	0.9789850																																																																																																																																																																																																																																																																																																																																																																		
C	-3.7923130	1.1439250	-0.9705000																																																																																																																																																																																																																																																																																																																																																																		
H	-1.7390150	1.4627280	-1.5164640																																																																																																																																																																																																																																																																																																																																																																		
C	-4.6942430	0.3283220	-0.2670750																																																																																																																																																																																																																																																																																																																																																																		
H	-4.9165630	-1.4197650	0.9777760																																																																																																																																																																																																																																																																																																																																																																		
H	-4.1609490	2.0039980	-1.5198860																																																																																																																																																																																																																																																																																																																																																																		
C	-6.0951790	0.6351240	-0.2697850																																																																																																																																																																																																																																																																																																																																																																		
N	-7.2314890	0.8846240	-0.2711790																																																																																																																																																																																																																																																																																																																																																																		
<p>exo-2-adduct (X=CN, Y=H)</p>  <p>E = -1296.45828587, H (0K) = -1296.114285,</p>	<p>Ylide S-3 (X=CN, Y=H)</p>  <p>E = -1296.43841764, H (0K) = -1296.098237,</p>																																																																																																																																																																																																																																																																																																																																																																				

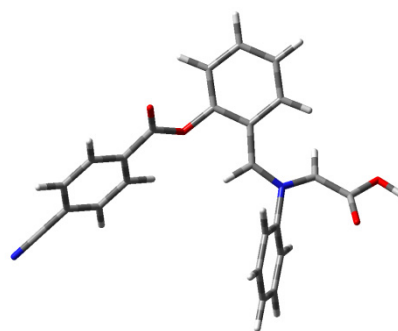
H (298K) = -1296.090847, G (298K) = -1296.167681 au.				H (298K) = -1296.072954, G (298K) = -1296.155181 au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	2.2872090	4.1276380	-0.8626540	C	2.5352930	-1.6106560	-0.0428830
C	3.1544600	3.6836420	0.1370700	C	1.4230450	-2.4843240	0.0292980
C	2.8439190	2.5282290	0.8587060	C	2.5297200	-0.1652600	-0.1256870
C	1.6849810	1.8102880	0.5741140	O	0.2264370	-0.8540440	-1.8510810
C	0.8214710	2.2746180	-0.4292070	C	-0.4090380	-1.2339230	-0.8933380
C	1.1099160	3.4323530	-1.1462770	O	0.1015200	-2.0534720	0.0791660
C	1.2254210	0.5495180	1.2731780	N	1.6887140	0.7037450	0.4497560
O	-0.1950020	0.6561410	1.4141410	C	0.7954820	0.4018230	1.4376840
C	-0.6646130	0.4707170	0.1049800	C	-0.3578130	1.2006580	1.7363390
O	-0.3502830	1.6074280	-0.7198560	O	-0.7539400	2.2246710	1.1930470
N	1.3609570	-0.6493800	0.4413440	O	-1.0573140	0.6415990	2.7842960
C	0.1893670	-0.7547400	-0.4047150	H	3.3622440	0.2988100	-0.6385080
C	-0.5326200	-2.0921630	-0.2112380	H	0.9371590	-0.5413490	1.9412380
O	-0.6037030	-2.7139520	0.8200240	H	-1.8219790	1.2330960	2.9033490
O	-1.1176320	-2.4849430	-1.3685790	C	1.5852560	-3.8663410	0.1130040
H	2.5213490	5.0271640	-1.4250750	C	2.8535840	-4.4360360	0.0761090
H	4.0635800	4.2344990	0.3580130	H	2.9657330	-5.5145510	0.1314800
H	3.5064360	2.1856080	1.6495790	C	3.9725110	-3.6070140	-0.0568750
H	0.4158280	3.7741810	-1.9074380	C	3.8080650	-2.2318990	-0.1166860
H	1.6574930	0.4137030	2.2664750	H	4.9700740	-4.0337010	-0.1041900
H	0.3989490	-0.6149020	-1.4710740	H	4.6814630	-1.5907500	-0.2025850
H	-1.5998640	-3.3103360	-1.1697370	H	0.6927460	-4.4801360	0.1827400
C	2.5737030	-1.2698540	0.1410850	C	1.8474300	2.0863530	0.0125480
C	2.6648290	-2.2039540	-0.9093870	C	2.2086910	3.0598500	0.9420740
C	3.7302170	-1.0079200	0.9019000	C	1.6952560	2.3867230	-1.3389230
C	3.8698510	-2.8497000	-1.1793630	C	2.4233580	4.3635830	0.5034700
H	1.7954890	-2.4364200	-1.5153550	H	2.3171730	2.7906040	1.9876290
C	4.9267470	-1.6608130	0.6182260	C	1.9075510	3.6988520	-1.7655750
H	3.6976450	-0.3012840	1.7236950	H	1.3890380	1.6065510	-2.0282560
C	5.0117040	-2.5856870	-0.4234820	C	2.2723720	4.6850590	-0.8487380
H	3.9094010	-3.5671770	-1.9948840	H	2.7097490	5.1299160	1.2179250
H	5.8024830	-1.4390150	1.2227310	H	1.7806920	3.9481870	-2.8151500
H	5.9483970	-3.0899730	-0.6405890	H	2.4368160	5.7050330	-1.1847740
C	-2.1677140	0.3021140	0.0976930	C	-1.8438530	-0.9196850	-0.6448560
C	-2.8074930	-0.2616230	1.2079280	C	-2.5305270	-1.3672260	0.4929860
C	-2.9179120	0.6794800	-1.0220900	C	-2.5149970	-0.1590600	-1.6126960
C	-4.1870620	-0.4419220	1.2033090	C	-3.8770320	-1.0640300	0.6568320
H	-2.2220350	-0.5564500	2.0705670	H	-2.0061530	-1.9378480	1.2490590
C	-4.2967060	0.4990390	-1.0347990	C	-3.8594980	0.1492960	-1.4546870
H	-2.4223820	1.1257980	-1.8763140	H	-1.9658240	0.1814130	-2.4834570
C	-4.9399040	-0.0631700	0.0802140	C	-4.5486270	-0.3056630	-0.3172470
H	-4.6858620	-0.8734630	2.0648230	H	-4.4147220	-1.4076780	1.5343620
H	-4.8808790	0.7936210	-1.9004080	H	-4.3825450	0.7385840	-2.2003730
C	-6.3621030	-0.2505300	0.0701140	C	-5.9389490	0.0040820	-0.1488690
N	-7.5151080	-0.4043770	0.0597010	N	-7.0671350	0.2523700	-0.0117010
TS Ylide S-3 (X=CN, Y=H) → <i>exo</i> -2-adduct (X=CN, Y=H) (TS _{S-3/exo-2})				Ylide S-3' (X=CN, Y=H)			



E = -1296.41838358, **H (0K)** = -1296.077633,
H (298K) = -1296.053901, **G (298K)** = -1296.130864
 au.

Imaginary frequency = 1.

C	2.3317930	-1.8011830	-0.2655100
C	1.2065350	-2.6252420	0.0149750
C	0.4809860	0.1006960	0.9412290
O	-0.6389790	2.2539050	1.0683780
C	-0.2838460	-0.7730580	-0.3937530
O	0.3193570	-0.5080670	-1.4861940
N	1.6924300	0.5555540	0.3110760
C	2.3084230	-0.3570030	-0.4386630
C	-0.3969370	1.1627400	1.5327990
O	-0.0545790	-2.1805570	0.0982800
O	-0.9812200	0.6987270	2.6670950
H	3.1138890	0.0523320	-1.0422060
H	0.7067700	-0.6567460	1.6889590
H	-1.6283010	1.3788690	2.9346380
C	1.3980830	-4.0058050	0.2008590
C	2.6582930	-4.5712870	0.0862970
H	2.7778980	-5.6413660	0.2326760
C	3.7693970	-3.7799190	-0.2433020
C	3.5933390	-2.4200320	-0.4303480
H	4.7521000	-4.2264180	-0.3567090
H	4.4452550	-1.7957690	-0.6898670
H	0.5230110	-4.6111930	0.4135960
C	1.9715880	1.9503000	0.0158540
C	2.5613370	2.7397550	1.0019550
C	1.6996180	2.4592410	-1.2542230
C	2.8819450	4.0653950	0.7107450
H	2.7698530	2.3171570	1.9804730
C	2.0306810	3.7845390	-1.5363430
H	1.2146080	1.8193790	-1.9838190
C	2.6191450	4.5877190	-0.5574270
H	3.3427470	4.6869610	1.4731190
H	1.8185810	4.1915840	-2.5209030
H	2.8715310	5.6203990	-0.7812200
C	-1.7907520	-0.5791610	-0.3557820
C	-2.6031890	-1.2187680	0.5888340
C	-2.3720200	0.2760930	-1.2979620
C	-3.9784430	-1.0086000	0.5920130
H	-2.1582660	-1.8909510	1.3132790
C	-3.7444170	0.4989710	-1.2992740
H	-1.7327960	0.7515550	-2.0328010
C	-4.5582510	-0.1439450	-0.3515380
H	-4.6096550	-1.5107990	1.3183560
H	-4.1939950	1.1626760	-2.0308630
C	-5.9747160	0.0791650	-0.3460830
N	-7.1240610	0.2611020	-0.3381180

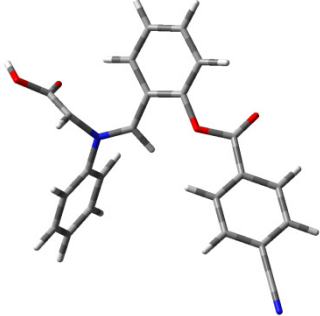
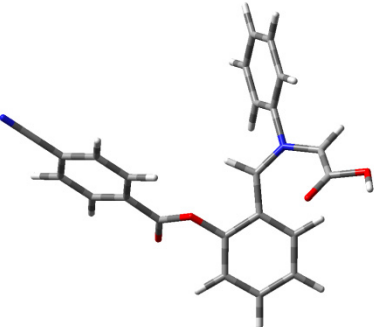


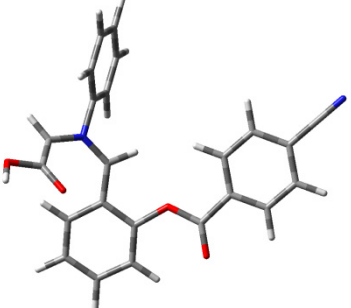
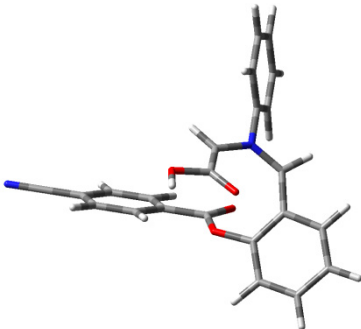
E = -1296.43860204, **H (0K)** = -1296.098119,
H (298K) = -1296.072720, **G (298K)** = -1296.156813
 au.

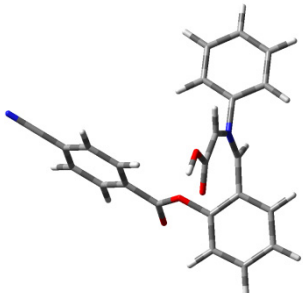
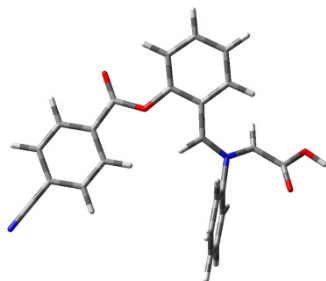
Imaginary frequency = 0.

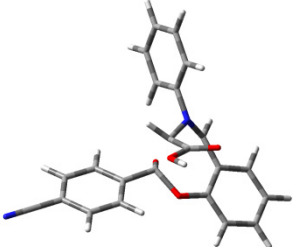
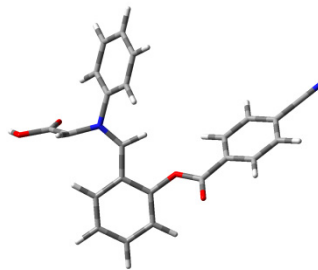
C	1.2643900	1.9144620	-0.0608360
C	-0.0209310	2.5104220	-0.1242900
C	1.3385630	0.4743070	0.0194610
O	-2.2917770	2.4931470	1.4664480
C	-2.1942240	1.7216210	0.5411410
O	-1.1071810	1.6434170	-0.2887310
N	2.4090920	-0.3168080	-0.1562180
C	3.5814350	0.0418650	-0.7589140
C	4.8272150	-0.6341850	-0.5330220
O	5.0728410	-1.5667390	0.2226980
O	5.8151740	-0.0692650	-1.3067350
H	0.4251840	-0.0619840	0.2268920
H	3.5614240	0.9338590	-1.3643910
H	6.6188320	-0.5684830	-1.0755880
C	-0.2105470	3.8855870	-0.1119530
C	0.8953180	4.7298200	-0.0176600
H	0.7527800	5.8061160	-0.0126600
C	2.1777870	4.1817920	0.0608440
C	2.3624310	2.8050900	0.0243250
H	3.0441050	4.8319860	0.1415120
H	3.3666750	2.4061290	0.0930000
H	-1.2146880	4.2877410	-0.1729550
C	2.2127880	-1.7043590	0.2505640
C	1.8157060	-1.9812670	1.5565010
C	2.3636130	-2.7201280	-0.6923880
C	1.5704730	-3.3045790	1.9261710
H	1.7241370	-1.1725420	2.2744270
C	2.1108640	-4.0360940	-0.3152650
H	2.6729100	-2.4718710	-1.7023060
C	1.7158730	-4.3310470	0.9929300
H	1.2728920	-3.5300300	2.9461110
H	2.2212220	-4.8333760	-1.0445620
H	1.5246160	-5.3603030	1.2830130
C	-3.2359630	0.7244060	0.1586960
C	-3.1106480	-0.1086120	-0.9622290
C	-4.3777160	0.6412650	0.9682370
C	-4.1162830	-1.0180800	-1.2703340
H	-2.2294230	-0.0391210	-1.5889550
C	-5.3854410	-0.2659080	0.6679330
H	-4.4565820	1.2964100	1.8290340
C	-5.2580740	-1.1014090	-0.4555950
H	-4.0267390	-1.6649130	-2.1367440
H	-6.2703370	-0.3356740	1.2917400
C	-6.2953070	-2.0405460	-0.7718400
N	-7.1358640	-2.8024730	-1.0283320

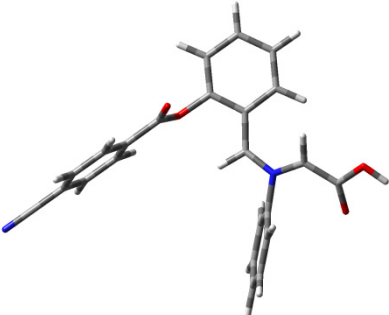
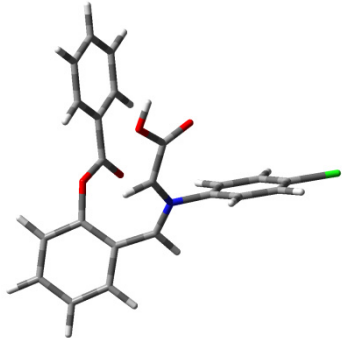
TS Ylide S-3 (X=CN, Y=H) → Ylide S-3' (X=CN, Y=H) (TS _{S-3/S-3'})				Ylide U-3'' (X=CN, Y=H)			
<p>E = -1296.43028654, H (0K) = -1296.090781, H (298K) = -1296.065981, G (298K) = -1296.147901 au.</p>				<p>E = -1296.43838011, H (0K) = -1296.097806, H (298K) = -1296.072529, G (298K) = -1296.155772 au.</p>			
Imaginary frequency = 1.				Imaginary frequency = 0.			
C	-1.6226530	2.0469950	-0.4849880	C	-1.6045870	-1.3912430	-0.5887450
C	-0.3927690	2.5913340	-0.0868730	C	-0.4208950	-2.1429870	-0.7935770
C	-1.7431350	0.6304940	-0.8930450	C	-1.4703070	0.0142520	-0.3085860
O	2.0815750	2.8606660	-1.2895270	O	1.6067490	-2.8965660	0.9192970
C	1.8617330	1.9193440	-0.5630490	C	1.7406130	-1.9192360	0.2226830
O	0.6665940	1.6924060	0.0609440	O	0.7995260	-1.4654830	-0.6623930
N	-2.0440410	-0.3481690	-0.0396680	N	-2.4105410	0.9218120	-0.0026660
C	-2.1407680	-0.2107860	1.3157790	C	-3.6573940	0.7280110	0.5462420
C	-2.8369990	-1.1410590	2.1561120	C	-3.9239130	-0.3005550	1.4983840
O	-3.4166360	-2.1788310	1.8554910	O	-3.1562720	-1.1717530	1.8983460
O	-2.7890990	-0.7167330	3.4648410	O	-5.2126990	-0.2139430	1.9753200
H	-1.5022790	0.3226680	-1.9021120	H	-0.4845090	0.4401570	-0.4280020
H	-1.8201730	0.7362460	1.7219790	H	-4.3613180	1.5343540	0.4072930
H	-3.2920330	-1.3919500	3.9542310	H	-5.2743570	-0.9282680	2.6342250
C	-0.2506430	3.9377380	0.2398650	C	-0.4386950	-3.4705920	-1.1936480
C	-1.3665580	4.7705260	0.1737230	C	-2.8257820	-2.0699530	-0.8056980
H	-1.2631840	5.8221610	0.4249480	C	-2.8513270	-3.3926730	-1.2303080
C	-2.6076710	4.2574330	-0.2079150	H	-3.8076430	-3.8786560	-1.4005070
C	-2.7307010	2.9076070	-0.5326670	C	-1.6631090	-4.1029080	-1.4123720
H	-3.4767840	4.9068990	-0.2549960	H	-1.6837370	-5.1452980	-1.7161190
H	-3.6918490	2.5021670	-0.8351070	H	0.4966220	-4.0016140	-1.3268310
H	0.7171790	4.3232570	0.5379540	H	-3.7566790	-1.5349430	-0.6747130
C	-2.1931620	-1.6685310	-0.6482850	C	-2.0508710	2.3067890	-0.2595390
C	-3.1750400	-1.8608730	-1.6153850	C	-2.2226920	3.2603920	0.7460120
C	-1.3059550	-2.6847730	-0.3008560	C	-1.5454250	2.6670740	-1.5100600
C	-3.2749280	-3.1036690	-2.2432900	C	-1.8728170	4.5862630	0.4955940
H	-3.8604630	-1.0544190	-1.8549440	H	-2.6101070	2.9532390	1.7118210
C	-1.4090720	-3.9183810	-0.9379120	C	-1.2011230	3.9975340	-1.7519510
H	-0.5534360	-2.5034610	0.4590800	H	-1.4485360	1.9143240	-2.2861520
C	-2.3934490	-4.1308610	-1.9073820	C	-1.3629520	4.9572390	-0.7513990
H	-4.0460580	-3.2662930	-2.9906740	H	-1.9920790	5.3288240	1.2792040
H	-0.7200890	-4.7161500	-0.6761700	H	-0.8188530	4.2840310	-2.7274750
H	-2.4728000	-5.0971500	-2.3972910	H	-1.0958370	5.9925840	-0.9429730
C	2.8504550	0.8518450	-0.2345420	C	2.9556260	-1.0508580	0.2153190
C	2.5634580	-0.1937090	0.6548890	C	3.1249970	0.0107390	-0.6843130
C	4.1079860	0.9241120	-0.8497290	C	3.9563690	-1.3370840	1.1543740
C	3.5263650	-1.1595690	0.9258630	C	4.2816180	0.7815420	-0.6443000
H	1.5911490	-0.2449800	1.1312840	H	2.3547100	0.2256500	-1.4155350
C	5.0733540	-0.0389090	-0.5861710	C	5.1128420	-0.5694760	1.2036350
H	4.3093660	1.7429560	-1.5319220	H	3.8071730	-2.1657820	1.8379640
C	4.7850910	-1.0871980	0.3051560	C	5.2803760	0.4959490	0.3018760
H	3.3139930	-1.9702330	1.6149920	H	4.4203840	1.6034030	-1.3389060
H	6.0477660	0.0104860	-1.0606550	H	5.8885050	-0.7850720	1.9309300

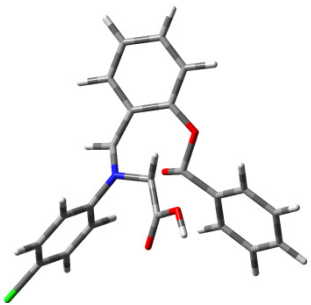
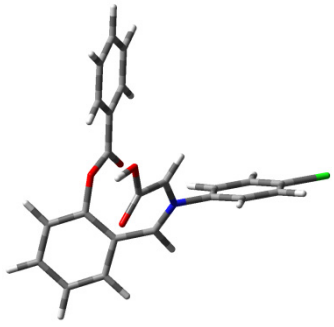
C	5.7775240	-2.0854670	0.5817350	C	6.4722470	1.2930330	0.3455870
N	6.5819610	-2.8952760	0.8052710	N	7.4378320	1.9406900	0.3798020
<p>TS Ylide S-3' (X=CN, Y=H) → Ylide U-3'' (X=CN, Y=H) (TS_{S-3'/U-3''})</p> 				<p>Ylide U-3' (X=CN, Y=H)</p> 			
<p>E = -1296.40876180, H (0K) = -1296.070070, H (298K) = -1296.044883, G (298K) = -1296.128347 au.</p>				<p>E = -1296.43954793, H (0K) = -1296.098843, H (298K) = -1296.073601, G (298K) = -1296.156744 au.</p>			
<p>Imaginary frequency = 1.</p>				<p>Imaginary frequency = 0.</p>			
C	-1.3265850	-1.6797560	0.0671640	C	1.5984010	-1.4902700	-0.2254590
C	-0.0897460	-2.3483640	-0.0239480	C	0.4039950	-2.2524300	-0.2248980
C	-1.3279660	-0.2349240	0.2029600	C	1.4830170	-0.0577080	-0.1505750
O	2.3424540	-2.7325780	1.2789380	O	-1.9164140	-2.3432380	-1.7544220
C	2.2045960	-1.8122890	0.5089910	C	-1.8808840	-1.6905050	-0.7371660
O	1.0336210	-1.5296880	-0.1538050	O	-0.7807080	-1.5642220	0.0652810
N	-2.2094830	0.5936600	-0.2808560	N	2.4431150	0.8734950	-0.0412780
C	-3.2480320	0.2148980	-1.2184260	C	3.7184610	0.7422920	0.4597320
C	-4.5160070	0.0254520	-0.6643480	C	4.0287210	-0.1352350	1.5405760
O	-4.7722130	-0.1742020	0.5409270	O	3.2766570	-0.9217080	2.1110320
O	-5.5379650	-0.0155600	-1.5940410	O	5.3438720	-0.0031110	1.9263400
H	-0.5162740	0.2171780	0.7685480	H	0.4927970	0.3575280	-0.2717460
H	-3.0591350	0.5016040	-2.2439200	H	4.4223200	1.5028960	0.1581950
H	-6.3181780	-0.2414770	-1.0579160	H	5.4363230	-0.6124320	2.6801890
C	-0.1871500	-3.7352970	-0.0992240	C	0.3949250	-3.6265460	-0.4171130
C	-1.2052230	-4.4680490	-0.0455450	C	2.8019700	-2.2043650	-0.4247460
H	-1.1570520	-5.5521330	-0.0979800	C	2.7980480	-3.5744110	-0.6543960
C	-2.4411780	-3.8283300	0.0852470	H	3.7395620	-4.0892230	-0.8221880
C	-2.5119440	-2.4403240	0.1336770	C	1.6004970	-4.2924910	-0.6387570
H	-3.3527730	-4.4136880	0.1534050	H	1.6003210	-5.3684520	-0.7855740
H	-3.4551850	-1.9284070	0.2983760	H	-0.5442900	-4.1659600	-0.3974340
H	0.9386800	-4.2307500	-0.1908110	H	3.7394510	-1.6643140	-0.4356580
C	-2.1564700	1.9714910	0.1736250	C	2.0766170	2.2087460	-0.4837260
C	-2.0856390	2.2469970	1.5410840	C	1.4722800	2.3800010	-1.7307530
C	-2.2139150	3.0059670	-0.7640300	C	2.3375650	3.3039230	0.3427260
C	-2.0454070	3.5748350	1.9711950	C	1.1160010	3.6627120	-2.1484870
H	-2.1183910	1.4318960	2.2571260	H	1.3069370	1.5185200	-2.3700580
C	-2.1559920	4.3251240	-0.3249150	C	1.9769660	4.5811400	-0.0834170
H	-2.3083280	2.7705490	-1.8182710	H	2.8009890	3.1431300	1.3104640
C	-2.0712740	4.6136050	1.0417670	C	1.3665390	4.7630960	-1.3271630
H	-2.0113120	3.7919460	3.0348920	H	0.6543510	3.8006630	-3.1218980
H	-2.1853020	5.1322670	-1.0511670	H	2.1662240	5.4343180	0.5615480
H	-2.0435550	5.6460150	1.3781700	H	1.0902700	5.7608560	-1.6560080
C	3.2690470	-0.8290750	0.1617060	C	-3.0309050	-0.9059630	-0.1981590
C	3.0834020	0.1871470	-0.7867260	C	-2.9642360	-0.2038350	1.0137520
C	4.4996120	-0.9535480	0.8228550	C	-4.2129330	-0.8909080	-0.9519550
C	4.1172850	1.0723850	-1.0701530	C	-4.0683070	0.5101630	1.4664930
H	2.1345500	0.2796530	-1.3017330	H	-2.0510870	-0.2224730	1.5969750
C	5.5360650	-0.0717300	0.5461740	C	-5.3192750	-0.1791430	-0.5068240
H	4.6244830	-1.7482200	1.5503260	H	-4.2444760	-1.4440430	-1.8844430
C	5.3480650	0.9474490	-0.4037860	C	-5.2506150	0.5265820	0.7072660

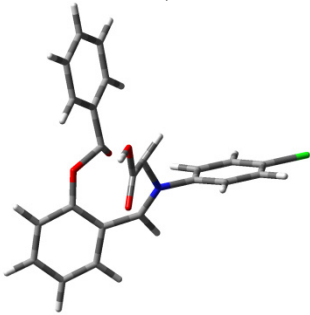
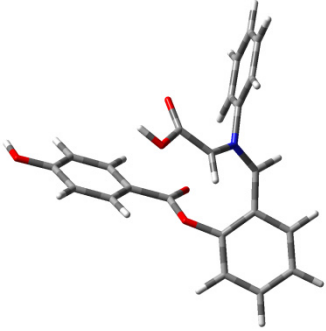
H	3.9815980	1.8601760	-1.8035890	H	-4.0245600	1.0549550	2.4037380
H	6.4894690	-0.1624980	1.0557610	H	-6.2362270	-0.1629550	-1.0865330
C	6.4142580	1.8621690	-0.6942880	C	-6.3891880	1.2653760	1.1717380
N	7.2780680	2.6045020	-0.9296750	N	-7.3119880	1.8656310	1.5473410
<p>TS Ylide U-3'' (X=CN, Y=H) → Ylide U-3' (X=CN, Y=H) (TS_{U-3''/U-3'})</p>  <p>E = -1296.43687771, H (0K) = -1296.096281, H (298K) = -1296.071879, G (298K) = -1296.151780 au.</p> <p>Imaginary frequency = 1.</p>				<p>Ylide U-3 (X=CN, Y=H)</p>  <p>E = -1296.44055151, H (0K) = -1296.100036, H (298K) = -1296.074943, G (298K) = -1296.155903 au.</p> <p>Imaginary frequency = 0.</p>			
C	-1.6417670	-1.4353740	-0.4507540	C	2.4892790	-1.1990540	-0.3574060
C	-0.4888560	-2.2583350	-0.5800400	C	1.4331570	-2.1360070	-0.3805110
C	-1.4585510	-0.0153760	-0.2957760	C	2.4012660	0.2277850	-0.1696540
O	2.1153020	-3.3606230	-0.0494960	O	0.0334050	-0.4289550	-2.0194230
C	1.9188400	-2.1681400	-0.1278760	C	-0.5141300	-0.9265750	-1.0598870
O	0.7238620	-1.5810990	-0.4098630	O	0.0984960	-1.7803110	-0.1894230
N	-2.3607510	0.9393500	-0.0209570	N	1.5000390	0.9800670	0.4786750
C	-3.5832890	0.8271490	0.6014690	C	0.5818410	0.6225500	1.4345350
C	-3.8365340	-0.1266430	1.6313210	C	0.7675030	-0.4829050	2.3164070
O	-3.0777190	-0.9940350	2.0564100	O	1.7285630	-1.2431270	2.3861870
O	-5.0992640	0.0332630	2.1562550	O	-0.3048160	-0.6210160	3.1754940
H	-0.4764710	0.3760080	-0.5137960	H	3.1957010	0.8113320	-0.6189730
H	-4.2700050	1.6431020	0.4360990	H	-0.2235750	1.3216240	1.5975610
H	-5.1526680	-0.6334410	2.8639410	H	-0.0423710	-1.3489530	3.7672800
C	-0.5815760	-3.6098660	-0.8983330	C	1.6612420	-3.4942420	-0.5807830
C	-2.8958180	-2.0605250	-0.6184980	C	3.7815400	-1.7104640	-0.6301450
C	-2.9949390	-3.4054000	-0.9514000	C	4.0160470	-3.0600090	-0.8411350
H	-3.9751240	-3.8523050	-1.0897050	H	5.0270820	-3.4092450	-1.0291360
C	-1.8431340	-4.1800310	-1.0838910	C	2.9507240	-3.9661020	-0.8031050
H	-1.9150640	-5.2375100	-1.3211130	H	3.1202240	-5.0266670	-0.9629840
H	0.3124490	-4.2078660	-0.9832510	H	0.8070430	-4.1637860	-0.5753840
H	-3.7949900	-1.4653760	-0.5251110	H	4.6141230	-1.0119250	-0.6453520
C	-1.9794690	2.2889110	-0.4054220	C	1.5050060	2.3911340	0.1235980
C	-2.0810510	3.3239680	0.5266280	C	1.6335160	3.3537610	1.1259650
C	-1.5200960	2.5336840	-1.7009720	C	1.3754570	2.7531450	-1.2180140
C	-1.7059440	4.6144380	0.1564310	C	1.6475930	4.7024470	0.7729830
H	-2.4352540	3.1058580	1.5286810	H	1.7353180	3.0399040	2.1597850
C	-1.1491960	3.8295130	-2.0624570	C	1.3880450	4.1067040	-1.5583620
H	-1.4777680	1.7198570	-2.4180430	H	1.2342480	1.9798420	-1.9664370
C	-1.2402860	4.8697040	-1.1361740	C	1.5262050	5.0798920	-0.5671000
H	-1.7711410	5.4200590	0.8819730	H	1.7603320	5.4580390	1.5450530
H	-0.8015100	4.0256940	-3.0725880	H	1.2774210	4.3986320	-2.5987190
H	-0.9530250	5.8778440	-1.4209750	H	1.5346340	6.1322620	-0.8366920
C	2.9927140	-1.1462570	0.0687650	C	-1.9505350	-0.7203720	-0.7112470
C	2.7441410	0.2325100	0.1126650	C	-2.5110310	-1.1664520	0.4941660
C	4.3028760	-1.6209900	0.2270660	C	-2.7506860	-0.0571180	-1.6523750
C	3.7907320	1.1269940	0.3058660	C	-3.8602430	-0.9527580	0.7531720
H	1.7326560	0.6047450	0.0085970	H	-1.8865200	-1.6481830	1.2360320
C	5.3550460	-0.7345480	0.4164720	C	-4.1004680	0.1539170	-1.4026390

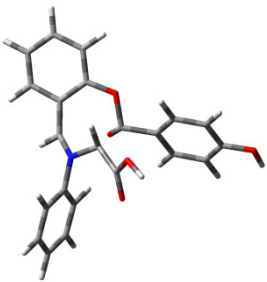
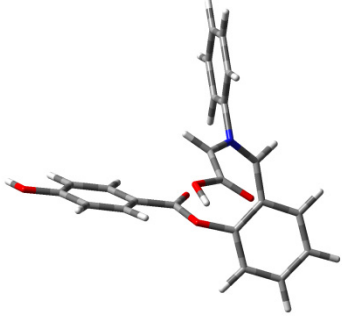
H	4.4754570	-2.6912020	0.1989220	H	-2.2967540	0.2829420	-2.5768320
C	5.1028910	0.6476970	0.4553520	C	-4.6626210	-0.2955920	-0.1952390
H	3.6016590	2.1946820	0.3438890	H	-4.2986190	-1.2863800	1.6878410
H	6.3698090	-1.0994860	0.5355120	H	-4.7246740	0.6621140	-2.1301920
C	6.1838050	1.5704890	0.6490290	C	-6.0555420	-0.0795360	0.0703910
N	7.0593660	2.3203430	0.8043450	N	-7.1854350	0.0957640	0.2845790
<p>TS Ylide U-3' (X=CN, Y=H) → Ylide U-3 (X=CN, Y=H) (TS_{U-3'/U-3})</p> 				<p>TS Ylide S-3' (X=CN, Y=H) → Ylide S-3'' (X=CN, Y=H) (TS_{S-3'/S-3''})</p> 			
<p>E = -1296.42481013, H (0K) = -1296.085226, H (298K) = -1296.060354, G (298K) = -1296.142917 au.</p>				<p>E = -1296.43641990, H (0K) = -1296.096065, H (298K) = -1296.071491, G (298K) = -1296.152555 au.</p>			
<p>Imaginary frequency = 1.</p>				<p>Imaginary frequency = 1.</p>			
C	2.1547730	-1.4461620	-0.4588370	C	1.2715000	1.9400400	0.2410380
C	1.0103980	-2.2507380	-0.3778160	C	0.0005600	2.5796100	0.2828030
C	2.0630090	0.0197380	-0.6260650	C	1.3167450	0.4948750	0.2388340
O	-1.2751290	-2.6342310	-1.9275290	O	-2.7547710	3.1741650	-0.2999410
C	-1.2771720	-1.8591020	-0.9979990	C	-2.3642550	2.0464140	-0.0936660
O	-0.2020410	-1.5825380	-0.2113050	O	-1.0833060	1.6994020	0.2137660
N	1.9189660	0.9824000	0.2833000	N	2.3401770	-0.3037500	-0.1017790
C	1.7632630	1.0262810	1.6441930	C	3.4470800	0.0656140	-0.8121430
C	1.5453560	-0.0705570	2.5351110	C	4.6852990	-0.6587480	-0.7800850
O	1.3713000	-1.2600970	2.2934960	O	4.9819770	-1.6506500	-0.1243480
O	1.5183590	0.3875820	3.8343550	O	5.5983760	-0.0665320	-1.6219980
H	2.1336640	0.3990170	-1.6388500	H	0.4279680	-0.0358740	0.5402200
H	1.8310020	2.0162230	2.0653860	H	3.3899130	1.0018060	-1.3445260
H	1.3498120	-0.4101310	4.3667380	H	6.4046980	-0.6032150	-1.5206590
C	1.0841970	-3.6381070	-0.3752350	C	-0.1263900	3.9592220	0.4242080
C	3.3971020	-2.0859890	-0.5593360	C	1.0241080	4.7453010	0.5135850
C	3.4917110	-3.4776970	-0.5532820	H	0.9231610	5.8220750	0.6117740
H	4.4654130	-3.9542200	-0.6207790	C	2.2865010	4.1535470	0.4696100
C	2.3346420	-4.2507060	-0.4629800	C	2.4076340	2.7768980	0.3260790
H	2.3990550	-5.3350570	-0.4608230	H	3.1815740	4.7641790	0.5446110
H	0.1780740	-4.2278480	-0.3052550	H	3.3946270	2.3307180	0.3117580
H	4.2946970	-1.4788160	-0.6378610	H	-1.1060810	4.4108380	0.4472750
C	1.9447870	2.3273150	-0.3014250	C	2.1507570	-1.7097690	0.2417720
C	3.1502140	2.8451430	-0.7674240	C	1.9105910	-2.0602170	1.5681100
C	0.7596650	3.0558680	-0.3760860	C	2.1468450	-2.6655940	-0.7730810
C	3.1661150	4.1251400	-1.3253850	C	1.6667570	-3.3977370	1.8844600
H	4.0577680	2.2554820	-0.6851250	H	1.9391090	-1.2979180	2.3400930
C	0.7857350	4.3313930	-0.9409680	C	1.8966910	-3.9959980	-0.4480150
H	-0.1624530	2.6214630	-0.0035240	H	2.3372920	-2.3609370	-1.7968510
C	1.9865910	4.8663380	-1.4137830	C	1.6578580	-4.3648660	0.8792120
H	4.1020300	4.5413620	-1.6864030	H	1.4920130	-3.6809580	2.9183640
H	-0.1337470	4.9048440	-1.0129430	H	1.8875370	-4.7467820	-1.2328230
H	2.0023950	5.8610710	-1.8497660	H	1.4687960	-5.4053470	1.1276930
C	-2.4641030	-1.0613730	-0.5655440	C	-3.2537360	0.8464550	-0.1409280
C	-2.4513010	-0.2716850	0.5934830	C	-2.7778140	-0.4677630	-0.0328520
C	-3.6184890	-1.1284320	-1.3567210	C	-4.6263850	1.0764710	-0.3148360
C	-3.5838280	0.4505910	0.9540550	C	-3.6615310	-1.5393200	-0.0925160
H	-1.5590210	-0.2375380	1.2083640				

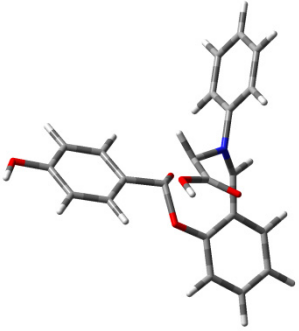
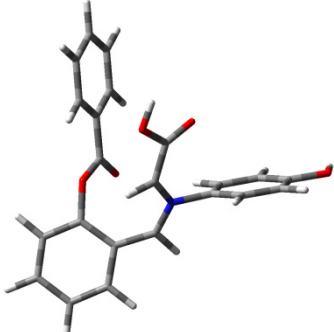
C	-4.7519330	-0.4064310	-1.0047340	H	-1.7176180	-0.6533950	0.0858910
H	-3.6074230	-1.7520470	-2.2442360	C	-5.5165820	0.0120790	-0.3717000
C	-4.7381710	0.3889800	0.1544750	H	-4.9763910	2.0990390	-0.4032430
H	-3.5850480	1.0600720	1.8518360	C	-5.0365920	-1.3043000	-0.2593980
H	-5.6480390	-0.4514020	-1.6148360	H	-3.2963670	-2.5577770	-0.0121040
C	-5.9042600	1.1392190	0.5222730	H	-6.5791860	0.1875470	-0.5026080
N	-6.8486660	1.7501160	0.8190050	C	-5.9496540	-2.4090620	-0.3170630
				N	-6.6894870	-3.3053930	-0.3632570
<p>TS Ylide U-3 (X=CN, Y=H) → <i>endo</i>-2-adduct (X=CN, Y=H) (TS_{U-3/<i>endo</i>-2})</p>  <p>E = -1296.42418246, H (0K) = -1296.083129, H (298K) = -1296.059527, G (298K) = -1296.136484 au.</p> <p>Imaginary frequency = 1.</p>				<p>TS Ylide S-3'' (X=CN, Y=H) → Ylide U-3' (X=CN, Y=H) (TS_{S-3''/U-3'})</p>  <p>E = -1296.41003000, H (0K) = -1296.071292, H (298K) = -1296.046104, G (298K) = -1296.129934 au.</p> <p>Imaginary frequency = 1.</p>			
C	2.4172200	-4.3922320	-0.5838870	C	-1.4492400	-1.7552380	0.1082190
C	3.5163500	-3.6040720	-0.9550900	C	-0.1953990	-2.3909590	-0.0805360
C	3.3772190	-2.2266070	-0.9822660	C	-1.4420990	-0.3092550	0.2227760
C	2.1682600	-1.5976950	-0.6100500	O	2.1309380	-2.6388730	1.3861060
C	1.0512130	-2.4112080	-0.2841920	C	2.0583430	-1.8020400	0.5193550
C	1.1992410	-3.8064980	-0.2694450	O	0.9261280	-1.5785620	-0.2348420
C	2.1677650	-0.1479870	-0.6320870	N	-2.4261810	0.5389580	0.3310700
O	0.1353630	-0.1792990	-1.5599310	C	-3.8280140	0.1744180	0.3726500
C	-0.4035990	-0.4750770	-0.4285580	C	-4.5888840	0.3856580	-0.7832590
O	-0.1643720	-1.9214300	-0.0038700	O	-4.1921610	0.7181070	-1.9160290
N	1.6279060	0.7222660	0.2256330	O	-5.9377960	0.1326810	-0.5880160
C	0.3474240	0.3701700	0.8083530	H	-0.4573000	0.1462420	0.2113330
C	0.4929160	-0.3923120	2.1050450	H	-4.2458480	0.1120640	1.3690910
O	1.5036020	-0.9213440	2.5089620	H	-6.3201350	0.2921920	-1.4684710
O	-0.6736510	-0.3994620	2.7922770	C	-0.0877230	-3.7703050	-0.2024870
H	4.2199980	-1.6029200	-1.2711580	C	-1.2412460	-4.5510290	-0.1348700
H	2.9548570	0.2933600	-1.2391460	H	-1.1575900	-5.6301020	-0.2286260
H	4.4614860	-4.0652550	-1.2232820	C	-2.4918760	-3.9547520	0.0463510
H	-0.2154010	1.2860050	0.9921950	C	-2.5983860	-2.5756420	0.1670790
H	2.5089580	-5.4748530	-0.5625240	H	-3.3868790	-4.5672700	0.0929520
H	0.3296400	-4.4064560	-0.0218910	H	-3.5532260	-2.0779970	0.2979270
H	-0.5116680	-0.9331810	3.5931360	H	0.8844880	-4.2247810	-0.3475310
C	1.9089840	2.1285790	0.0386960	C	-2.0701810	1.9459020	0.4846130
C	2.4321130	2.8521800	1.1116650	C	-1.2616230	2.3343890	1.5558490
C	1.6435490	2.7435960	-1.1875050	C	-2.5705190	2.8833070	-0.4249750
C	2.7012620	4.2115650	0.9503970	C	-0.9431510	3.6844700	1.7191120
H	2.6348630	2.3453570	2.0504370	H	-0.9121950	1.5941260	2.2705910
C	1.9250560	4.1021610	-1.3393280	C	-2.2347150	4.2239620	-0.2523840
H	1.2002690	2.1571100	-1.9861260	H	-3.1900800	2.5363000	-1.2464850
C	2.4521110	4.8357480	-0.2742890	C	-1.4252730	4.6295290	0.8145040
H	3.1133390	4.7799280	1.7792310	H	-0.3255080	3.9921520	2.5582570
H	1.7211430	4.5888690	-2.2888840	H	-2.6070550	4.9588680	-0.9606260
H	2.6655660	5.8938090	-0.3968890	H	-1.1763250	5.6794360	0.9408530
C	-1.9169310	-0.2870700	-0.3485490	C	3.1554610	-0.8731030	0.1327680
C	-2.7426650	-1.0705520	0.4655190	C	3.0458290	0.0266640	-0.9374840
C	-2.4865230	0.7204820	-1.1366650	C	4.3387910	-0.9289550	0.8837290

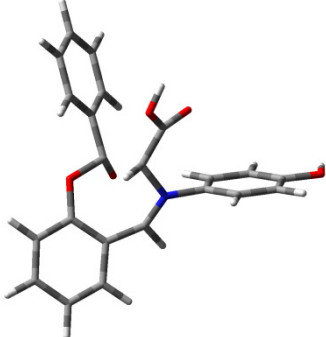
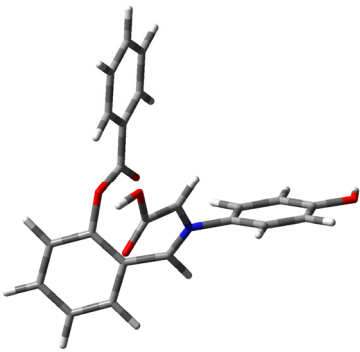
C	-4.1159500	-0.8467880	0.4983370	C	4.1088420	0.8657790	-1.2524530
H	-2.3100760	-1.8603490	1.0658000	H	2.1348900	0.0646610	-1.5232610
C	-3.8555340	0.9587610	-1.1044380	C	5.4033850	-0.0925140	0.5756630
H	-1.8414020	1.2995940	-1.7879660	H	4.4053260	-1.6343480	1.7049240
C	-4.6818590	0.1739350	-0.2823980	C	5.2917220	0.8105960	-0.4961630
H	-4.7564510	-1.4589190	1.1254060	H	4.0318870	1.5634660	-2.0795690
H	-4.2940100	1.7398420	-1.7174260	H	6.3205270	-0.1298830	1.1538650
C	-6.0954970	0.4107790	-0.2442700	C	6.3884770	1.6771780	-0.8188850
N	-7.2423910	0.6050470	-0.2114030	N	7.2780430	2.3795710	-1.0793600
Ylide S-3" (X=CN, Y=H)				Ylide S-3 (X=H, Y=Cl)			
							
<p>E = -1296.43844712, H (0K) = -1296.098040, H (298K) = -1296.072603, G (298K) = -1296.157445 au.</p>				<p>E = -1663.79192893, H (0K) = -1663.459904, H (298K) = -1663.435207, G (298K) = -1663.516192 au.</p>			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	1.2856820	1.8966590	-0.4033860	C	-1.4114100	-2.4993620	-0.0737430
C	0.0275300	2.5324010	-0.5403130	C	-2.5663270	-1.6813470	-0.1065360
C	1.3085800	0.4547110	-0.3273880	C	-0.0303770	-2.0663880	-0.0243960
O	-1.5329750	2.0995050	1.6359350	O	-1.2370680	-0.0629820	-1.8954580
C	-1.8444060	1.5913960	0.5854770	C	-1.8515070	0.4409530	-0.9810650
O	-1.1295780	1.7391020	-0.5752610	O	-2.5276510	-0.2945730	-0.0356700
N	2.3193150	-0.3441680	0.0499370	N	0.4904320	-1.0253250	0.6390630
C	3.4346430	0.0427210	0.7358200	C	-0.1436570	-0.3085830	1.6136980
C	4.6642570	-0.6981210	0.7288890	C	0.2355070	1.0225870	1.9888360
O	4.9458700	-1.7188850	0.1124790	O	1.1466880	1.7194580	1.5570530
O	5.5881150	-0.0827180	1.5415840	O	-0.6070970	1.4930260	2.9715400
H	0.4029640	-0.0724490	-0.5876370	H	0.7035780	-2.6995010	-0.5061720
H	3.3901950	0.9978560	1.2342800	H	-1.0461640	-0.7413530	2.0153630
H	6.3875980	-0.6327690	1.4594440	H	-0.2909070	2.3981390	3.1427520
C	-0.1082060	3.9003280	-0.7151120	C	-3.8456050	-2.2320200	-0.1589020
C	1.0300440	4.7053070	-0.7679730	C	-4.0231740	-3.6103480	-0.2306520
H	0.9302860	5.7788410	-0.8954990	H	-5.0249530	-4.0261930	-0.2812710
C	2.2906910	4.1155920	-0.6506140	C	-2.9015110	-4.4450690	-0.2602770
C	2.4189840	2.7442040	-0.4611360	C	-1.6305560	-3.8947930	-0.1854830
H	3.1853560	4.7295220	-0.7007620	H	-3.0199250	-5.5223130	-0.3318370
H	3.4098860	2.3141990	-0.3845550	H	-0.7616110	-4.5477560	-0.1917430
H	-1.1034100	4.3230040	-0.8088860	H	-4.6921030	-1.5526010	-0.1660050
C	2.1073470	-1.7621200	-0.2225680	C	1.8777420	-0.7295510	0.3115280
C	2.0948930	-2.6656640	0.8389150	C	2.8535980	-0.8092280	1.3027880
C	1.8584520	-2.1750700	-1.5290680	C	2.2071060	-0.4296360	-1.0077170
C	1.8280930	-4.0075040	0.5813990	C	4.1859770	-0.5897420	0.9692510
H	2.2901680	-2.3122100	1.8459660	H	2.5675590	-1.0404080	2.3234080
C	1.5983660	-3.5236010	-1.7774800	C	3.5415720	-0.2024340	-1.3448270
H	1.8929030	-1.4523170	-2.3379560	H	1.4197060	-0.3484030	-1.7501010
C	1.5815590	-4.4391430	-0.7251550	C	4.5171170	-0.2871620	-0.3535500
H	1.8110350	-4.7177930	1.4028840	H	4.9620050	-0.6527360	1.7240210
H	1.4166700	-3.8562490	-2.7953570	H	3.8184640	0.0440630	-2.3639150
H	1.3790180	-5.4883060	-0.9209200	C	-2.0069440	1.9004210	-0.7522370
C	-3.0441120	0.7276150	0.3822500	C	-2.7045100	2.4258920	0.3455350

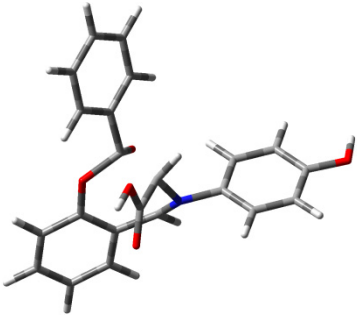
C	-3.3946750	0.2051010	-0.8704560	C	-1.4374350	2.7666250	-1.6967740
C	-3.8354190	0.4461880	1.5046580	C	-2.8310390	3.8061430	0.4883860
C	-4.5254190	-0.5937030	-1.0004870	H	-3.1299960	1.7565210	1.0833230
H	-2.7835480	0.4280460	-1.7371450	C	-1.5668800	4.1442620	-1.5486190
C	-4.9652720	-0.3522880	1.3832140	H	-0.9007460	2.3411330	-2.5380300
H	-3.5474510	0.8630860	2.4636680	C	-2.2652080	4.6656740	-0.4564200
C	-5.3151900	-0.8769080	0.1266420	H	-3.3707120	4.2117860	1.3396530
H	-4.8038890	-1.0009520	-1.9667810	H	-1.1232610	4.8117120	-2.2819180
H	-5.5805450	-0.5746830	2.2486880	H	-2.3662180	5.7415460	-0.3403870
C	-6.4807780	-1.7025500	-0.0063600	Cl	6.2004960	-0.0092430	-0.7743080
N	-7.4253930	-2.3724280	-0.1150710				
<p>TS Ylide S-3 (X=H, Y=Cl) → <i>exo</i>-2-adduct (X=H, Y=Cl)</p>  <p>E = -1663.76835052, H (0K) = -1663.436055, H (298K) = -1663.412836, G (298K) = -1663.488919 au.</p> <p>Imaginary frequency = 1.</p>				<p>Ylide U-3 (X=H, Y=Cl)</p>  <p>E = -1663.79337409, H (0K) = -1663.461132, H (298K) = -1663.436603, G (298K) = -1663.516498 au.</p> <p>Imaginary frequency = 0.</p>			
C	-1.4364540	-2.4612370	-0.2176940	C	-1.4090690	-2.1939700	-0.4384720
C	-2.6436560	-1.7221820	-0.0586340	C	-2.4729540	-1.2682170	-0.5146520
C	-0.0993650	-1.9025070	-0.2995210	C	-0.0275570	-1.9189960	-0.1343390
O	-0.9166080	-0.1377470	-1.4909700	O	-0.8452440	0.3946030	-1.9713460
C	-1.4727280	0.3596470	-0.4605280	C	-1.4924510	0.8494170	-1.0520940
O	-2.7179020	-0.3884780	-0.0259440	O	-2.3147560	0.0905890	-0.2616190
N	0.4492900	-0.9455180	0.4475260	N	0.5355690	-0.9434410	0.5952580
C	-0.4711080	0.0248610	0.9773300	C	-0.0182050	-0.1278260	1.5505240
C	0.1386990	1.2562380	1.5711220	C	-1.1472220	-0.5045530	2.3364160
O	1.1021090	1.8661310	1.1626010	O	-1.7603200	-1.5680470	2.3187440
O	-0.5974170	1.6714150	2.6334430	O	-1.5000970	0.4990700	3.2145130
H	0.6315910	-2.5175410	-0.8172640	H	0.6957040	-2.6075810	-0.5548330
H	-1.1436210	-0.4452440	1.6912450	H	0.5265630	0.7765570	1.7726720
H	-0.2371780	2.5429040	2.8847320	H	-2.2304180	0.1148910	3.7318870
C	-3.8606910	-2.4206550	0.0542120	C	-3.7678370	-1.6683070	-0.8330480
C	-3.8994690	-3.8032700	-0.0206310	C	-1.7181010	-3.5328070	-0.7806530
H	-4.8539110	-4.3156040	0.0663970	C	-3.0028230	-3.9359740	-1.1090110
C	-2.7244860	-4.5415480	-0.2357470	H	-3.1976700	-4.9774090	-1.3478740
C	-1.5212700	-3.8687590	-0.3471980	C	-4.0431660	-3.0005740	-1.1232150
H	-2.7584570	-5.6231890	-0.3188950	H	-5.0553300	-3.3028020	-1.3751870
H	-0.6036020	-4.4277010	-0.5158160	H	-4.5441640	-0.9104280	-0.8644780
H	-4.7654760	-1.8343320	0.1769430	H	-0.9151300	-4.2650240	-0.7555460
C	1.8576470	-0.6745030	0.2281810	C	1.9486490	-0.7257740	0.3429300
C	2.7589330	-0.8992690	1.2670700	C	2.8545830	-0.7581650	1.4036730
C	2.2972720	-0.2478600	-1.0250650	C	2.3769920	-0.4796500	-0.9622030
C	4.1211770	-0.6949040	1.0560630	C	4.2108560	-0.5594710	1.1563410
H	2.3993950	-1.2360810	2.2346480	H	2.4964140	-0.9524750	2.4092810
C	3.6591990	-0.0481310	-1.2424290	C	3.7337790	-0.2760090	-1.2126000
H	1.5639860	-0.0552580	-1.8011010	H	1.6442550	-0.4149920	-1.7602730
C	4.5579020	-0.2726680	-0.1996020	C	4.6376930	-0.3213080	-0.1516160
H	4.8362180	-0.8671540	1.8528850	H	4.9311060	-0.5968640	1.9661670
H	4.0193450	0.2881930	-2.2085300	H	4.0836220	-0.0712770	-2.2184490
C	-1.8770630	1.8234500	-0.4924560				

C	-2.8137300	2.3591890	0.3995510	C	-1.5262050	2.2861880	-0.6669940
C	-1.2825720	2.6553270	-1.4462290	C	-2.1897080	2.7515330	0.4779250
C	-3.1504180	3.7117350	0.3337870	C	-0.8654020	3.1935460	-1.5079200
H	-3.2860820	1.7157150	1.1336410	C	-2.1886960	4.1139400	0.7711990
C	-1.6155170	4.0083440	-1.5060680	H	-2.6770920	2.0488350	1.1428050
H	-0.5712070	2.2238470	-2.1416200	C	-0.8720750	4.5538210	-1.2120980
C	-2.5506720	4.5406380	-0.6165640	H	-0.3573200	2.8130880	-2.3878740
H	-3.8862350	4.1169450	1.0239120	C	-1.5348240	5.0157720	-0.0719450
H	-1.1485680	4.6455600	-2.2526080	H	-2.6958820	4.4719360	1.6627100
H	-2.8143030	5.5940480	-0.6662010	H	-0.3619520	5.2535220	-1.8682890
Cl	6.2754030	-0.0216860	-0.4718700	H	-1.5392350	6.0774000	0.1608680
				Cl	6.3466670	-0.0669830	-0.4642120
<p>TS Ylide U-3 (X=H, Y=Cl) → <i>endo</i>-2-adduct (X=H, Y=Cl)</p>  <p>E = -1663.77431420, H (0K) = -1663.442259, H (298K) = -1663.418834, G (298K) = -1663.495559 au.</p> <p>Imaginary frequency = 1.</p>				<p>Ylide S-3 (X=OH, Y=H)</p>  <p>E = -1279.41515716, H (0K) = -1279.069343, H (298K) = -1279.044721, G (298K) = -1279.124843 au.</p> <p>Imaginary frequency = 0.</p>			
C	-1.2300750	-2.3226060	-0.4184780	C	2.3160020	-1.6813780	-0.0631470
C	-2.4296620	-1.5478720	-0.3780730	C	1.1631660	-2.4969790	0.0375110
C	0.1141950	-1.8721640	-0.2175870	C	2.3626420	-0.2370450	-0.1601600
O	-2.4912650	-0.2216370	-0.2392590	O	-0.0096190	-0.9308580	-1.8962800
C	-0.9668000	-0.0820170	2.0820120	C	-0.6448550	-1.2245990	-0.9064650
O	-0.6935110	0.2025000	-1.6637660	O	-0.1270220	-1.9909140	0.1159260
N	0.6071110	-0.7911380	0.3660880	N	1.5805610	0.6622800	0.4514950
C	-0.2106180	0.2716250	0.8581550	C	0.7382460	0.3982490	1.4936180
C	-1.3074860	0.6009740	-0.6564220	C	-0.3818230	1.2248610	1.8353340
O	-1.2259850	-1.2049520	2.4730700	O	-0.7689600	2.2642250	1.3135380
O	-1.3798630	1.0312570	2.7438880	O	-1.0568440	0.6827230	2.9084770
H	0.8850630	-2.5778620	-0.5150310	H	3.1809150	0.1945110	-0.7220820
H	0.3752040	1.1780990	0.9760570	H	0.8678930	-0.5536640	1.9835110
H	-1.9138200	0.7053310	3.4920740	H	-1.8045130	1.2906860	3.0488770
C	-3.6696330	-2.2038230	-0.4902910	C	1.2604950	-3.8846780	0.1233080
C	-1.3496810	-3.7183900	-0.6677150	C	2.4996130	-4.5153990	0.0627080
C	-2.5728970	-4.3424700	-0.7913240	H	2.5608810	-5.5980140	0.1210370
H	-2.6292260	-5.4120370	-0.9666090	C	3.6543030	-3.7427120	-0.0966260
C	-3.7439070	-3.5717030	-0.6843130	C	3.5557720	-2.3605460	-0.1593580
H	-4.7169400	-4.0463630	-0.7781190	H	4.6288450	-4.2179240	-0.1616170
H	-4.5626670	-1.5892070	-0.4472310	H	4.4570060	-1.7622190	-0.2655730
H	-0.4371630	-4.3056220	-0.7365550	H	0.3409960	-4.4542130	0.2152460
C	2.0200790	-0.5343430	0.2111810	C	1.7536380	2.0334590	-0.0122950
C	2.8372030	-0.4621240	1.3405570	C	2.1866800	3.0105280	0.8820140
C	2.5413060	-0.3406670	-1.0691710	C	1.5434550	2.3177050	-1.3595560
C	4.1998300	-0.2154480	1.1881190	C	2.4160680	4.3006350	0.4118310
H	2.4112850	-0.6127440	2.3277420	H	2.3379010	2.7535340	1.9252890
C	3.9054050	-0.0954280	-1.2246820	C	1.7712550	3.6165300	-1.8180270
H	1.8649100	-0.3441750	-1.9178690	H	1.1823340	1.5351100	-2.0192590
C	4.7217230	-0.0388550	-0.0951370	C	2.2083700	4.6057670	-0.9367660
H	4.8524500	-0.1667410	2.0527450	H	2.7586280	5.0693440	1.0986310

H	4.3279160	0.0634500	-2.2107950	H	1.6004170	3.8530350	-2.8644350
C	-1.7270260	2.0534940	-0.5313670	H	2.3854270	5.6152770	-1.2974640
C	-2.7788530	2.4895740	0.2816270	C	-2.0513300	-0.8516960	-0.6453540
C	-1.0125460	2.9885800	-1.2895980	C	-2.7336940	-1.2023840	0.5325140
C	-3.1074640	3.8449360	0.3339250	C	-2.7281090	-0.1259410	-1.6361910
H	-3.3425200	1.7704210	0.8631290	C	-4.0599350	-0.8371630	0.7139810
C	-1.3357430	4.3431360	-1.2277680	H	-2.2147920	-1.7492760	1.3103490
H	-0.2162370	2.6317990	-1.9346060	C	-4.0553190	0.2421570	-1.4623520
C	-2.3857470	4.7759180	-0.4149330	H	-2.1955020	0.1421540	-2.5423730
H	-3.9316220	4.1734630	0.9621640	C	-4.7255300	-0.1121530	-0.2836290
H	-0.7747870	5.0597430	-1.8224230	H	-4.5980830	-1.0990190	1.6192200
H	-2.6431160	5.8310400	-0.3693760	H	-4.5738980	0.8061440	-2.2353690
Cl	6.4386380	0.2705930	-0.2871570	O	-6.0265300	0.2171270	-0.0530320
				H	-6.3612490	0.7368310	-0.8008510
<p>TS Ylide S-3 (X=OH, Y=H) → <i>exo</i>-2-adduct (X=OH, Y=H)</p>  <p>E = -1279.38994818, H (0K) = -1279.043923, H (298K) = -1279.020762, G (298K) = -1279.095926 au.</p> <p>Imaginary frequency = 1.</p>				<p>Ylide U-3 (X=OH, Y=H)</p>  <p>E = -1279.41675446, H (0K) = -1279.070707, H (298K) = -1279.046236, G (298K) = -1279.125482 au.</p> <p>Imaginary frequency = 0.</p>			
C	-2.0802710	1.8980770	-0.2507210	C	2.4095220	-1.0062850	-0.4085180
C	-0.9089270	2.6619500	0.0183870	C	1.4203980	-2.0126530	-0.3871950
C	-2.1379400	0.4554630	-0.4183410	C	2.2077690	0.4100030	-0.2280770
O	-0.1403960	0.4999670	-1.4911140	O	-0.1693330	-0.5953460	-2.0964830
C	0.4911080	0.7321500	-0.4099060	C	-0.6463710	-1.0263810	-1.0672740
O	0.3258250	2.1563520	0.0901240	O	0.0799390	-1.7318130	-0.1396300
N	-1.5574490	-0.4876750	0.3209480	N	1.2815580	1.0813140	0.4744060
C	-0.3195480	-0.0981320	0.9414000	C	0.4779590	0.6592540	1.5029170
C	0.5043810	-1.2022610	1.5268730	C	0.8113070	-0.4253530	2.3649610
O	0.6801410	-2.3094330	1.0689520	O	1.8363460	-1.1011310	2.3756260
O	1.1269950	-0.7668310	2.6530250	O	-0.1899680	-0.6508840	3.2896790
H	-2.9728760	0.0882520	-1.0088650	H	2.9119280	1.0593740	-0.7344930
H	-0.4989430	0.6728950	1.6874650	H	-0.3922450	1.2657750	1.6997310
H	1.7513800	-1.4738260	2.9031530	H	0.1656950	-1.3606350	3.8539570
C	-1.0299380	4.0518530	0.2066430	C	1.7347260	-3.3516220	-0.5977800
C	-2.2591660	4.6821540	0.1018760	C	3.7224710	-1.4227600	-0.7322840
H	-2.3218160	5.7570820	0.2494040	C	4.0418030	-2.7539310	-0.9532220
C	-3.4130730	3.9499280	-0.2195800	H	5.0665560	-3.0325570	-1.1815090
C	-3.3089390	2.5829850	-0.4063350	C	3.0449070	-3.7319870	-0.8729570
H	-4.3720910	4.4471060	-0.3256370	H	3.2822690	-4.7784340	-1.0405010
H	-4.1943730	2.0033270	-0.6575890	H	0.9306400	-4.0796680	-0.5582420
H	-0.1226250	4.6102510	0.4129280	H	4.5022860	-0.6669980	-0.7804160
C	-1.9089620	-1.8650050	0.0228860	C	1.1155990	2.4754970	0.0954500
C	-2.5409820	-2.6246510	1.0061260	C	1.2205160	3.4731790	1.0654430
C	-1.6634860	-2.3847370	-1.2482280	C	0.8471510	2.7852340	-1.2386200
C	-2.9327400	-3.9301860	0.7112000	C	1.0686910	4.8062160	0.6859570
H	-2.7261760	-2.1939980	1.9858090	H	1.4318360	3.1986370	2.0938590
C	-2.0654670	-3.6894360	-1.5342300	C	0.6937020	4.1232120	-1.6055540
H	-1.1427210	-1.7690200	-1.9739560	H	0.7303280	1.9800620	-1.9575780
C	-2.6978430	-4.4624460	-0.5583390	C	0.8065320	5.1323950	-0.6475030

H	-3.4269710	-4.5281210	1.4716730	H	1.1623090	5.5905860	1.4315850
H	-1.8745760	-4.1046930	-2.5198210	H	0.4744990	4.3735170	-2.6395930
H	-3.0059220	-5.4792920	-0.7853930	H	0.6863540	6.1725740	-0.9374010
C	1.9836580	0.4691670	-0.3780800	C	-2.0649850	-0.8885760	-0.6654780
C	2.8284970	1.0255700	0.5916730	C	-2.5472410	-1.2650400	0.6002500
C	2.5356950	-0.3658200	-1.3523670	C	-2.9579500	-0.3579450	-1.6073020
C	4.1937780	0.7558610	0.5888380	C	-3.8911970	-1.1159830	0.9134290
H	2.4166300	1.6855840	1.3471750	H	-1.8607050	-1.6453090	1.3472150
C	3.9001280	-0.6479280	-1.3607800	C	-4.3055780	-0.2130850	-1.3033200
H	1.8834770	-0.7839280	-2.1110470	H	-2.5770940	-0.0667540	-2.5806520
C	4.7338960	-0.0868300	-0.3885950	C	-4.7764460	-0.5942320	-0.0394480
H	4.8552410	1.1923860	1.3308510	H	-4.2754620	-1.3922360	1.8898920
H	4.3179120	-1.2997020	-2.1266950	H	-4.9945060	0.1935630	-2.0414920
O	6.0818430	-0.3232380	-0.3447140	O	-6.0849460	-0.4770990	0.3207820
H	6.3181810	-0.9114580	-1.0786730	H	-6.5916160	-0.1254490	-0.4282330
TS Ylide U-3 (X=OH, Y=H) → <i>endo</i>-2-adduct (X=OH, Y=H)				Ylide S-3 (X=H, Y=OH)			
							
E = -1279.39528867, H (0K) = -1279.048927, H (298K) = -1279.025918, G (298K) = -1279.101057 au.				E = -1279.41323897, H (0K) = -1279.067490, H (298K) = -1279.042818, G (298K) = -1279.123540 au.			
Imaginary frequency = 1.				Imaginary frequency = 0.			
C	1.8343520	-4.5673810	-0.5798410	C	-1.1443820	-2.4984740	-0.0615670
C	3.0062390	-3.8866910	-0.9437830	C	-2.2939710	-1.6735720	-0.0368370
C	2.9997340	-2.5026910	-0.9623780	C	0.2395290	-2.0718410	-0.0699840
C	1.8555840	-1.7605450	-0.5906820	O	-1.1131520	-0.0606300	-1.9226020
C	0.6608090	-2.4639050	-0.2752160	C	-1.6436370	0.4448230	-0.9581440
C	0.6779230	-3.8689290	-0.2668980	O	-2.2348430	-0.2868260	0.0443260
C	2.0008320	-0.3200460	-0.6022040	N	0.7951030	-1.0382060	0.5782990
O	-0.5016530	-1.8656830	-0.0020220	C	0.2086260	-0.3397200	1.5945330
C	-0.6122810	-0.3914110	-0.4398520	C	0.5897680	0.9901730	1.9715560
O	-0.0318490	-0.1553540	-1.5611100	O	1.4693800	1.7100250	1.5136140
N	1.5278280	0.6014870	0.2403610	O	-0.2154320	1.4340730	3.0003290
C	0.2123980	0.3758170	0.8085220	H	0.9489990	-2.7044620	-0.5875700
C	0.2769270	-0.3930630	2.1058550	H	-0.6690400	-0.7851770	2.0359740
O	1.2264910	-1.0257210	2.5120750	H	0.1023760	2.3380940	3.1739110
O	-0.8812540	-0.2770580	2.7989490	C	-3.5784960	-2.2129420	-0.0398590
H	1.8215840	-5.6540780	-0.5638980	C	-3.7698560	-3.5895130	-0.1178700
H	3.9037850	-4.4351550	-1.2115840	H	-4.7759600	-3.9978210	-0.1299290
H	3.9001890	-1.9614750	-1.2439880	C	-2.6564310	-4.4311790	-0.2031240
H	-0.2467250	-4.3833170	-0.0261250	C	-1.3788640	-3.8910140	-0.1765190
H	2.8391800	0.0427260	-1.1926830	H	-2.7857380	-5.5069130	-0.2799600
H	-0.2634220	1.3409050	0.9839530	H	-0.5159720	-4.5502260	-0.2254010
H	-0.7692830	-0.8282330	3.5963740	H	-4.4191960	-1.5271770	-0.0037140
C	1.9409990	1.9733300	0.0472730	C	2.1613330	-0.7346030	0.1838640
C	2.5327620	2.6506980	1.1147350	C	3.1893820	-0.7961950	1.1261250
C	1.7318540	2.6036790	-1.1821140	C	2.4295190	-0.4379760	-1.1492770
C	2.9301620	3.9771370	0.9444780	C	4.4987030	-0.5656670	0.7303500
H	2.6873400	2.1325530	2.0565060	H	2.9553850	-1.0260670	2.1603840
C	2.1410040	3.9282550	-1.3429320	C	3.7440430	-0.1978390	-1.5468740

H	1.2313240	2.0553550	-1.9741640	H	1.6096190	-0.3681470	-1.8570110
C	2.7386870	4.6147000	-0.2837190	C	4.7795000	-0.2615340	-0.6093470
H	3.3963320	4.5088930	1.7690610	H	5.3173600	-0.6132990	1.4406810
H	1.9814510	4.4267520	-2.2949430	H	3.9601630	0.0484770	-2.5844980
H	3.0516330	5.6469600	-0.4133730	C	-1.7751430	1.9056980	-0.7187230
C	-2.1006040	-0.0728950	-0.3693360	C	-2.3509640	2.4338500	0.4461400
C	-2.9932240	-0.7446490	0.4698990	C	-1.3123420	2.7690130	-1.7221470
C	-2.5915710	0.9494050	-1.1918990	C	-2.4621310	3.8146020	0.5977410
C	-4.3447000	-0.3999030	0.4915420	H	-2.6913110	1.7665350	1.2285630
H	-2.6367700	-1.5483980	1.1017480	C	-1.4278670	4.1470740	-1.5658380
C	-3.9350020	1.3081800	-1.1709450	H	-0.8691630	2.3404610	-2.6148130
H	-1.9042270	1.4507730	-1.8649740	C	-2.0039640	4.6714510	-0.4058030
C	-4.8189240	0.6309430	-0.3246080	H	-2.9060400	4.2226710	1.5015860
H	-5.0320520	-0.9373230	1.1434920	H	-1.0684920	4.8127530	-2.3455280
H	-4.3183350	2.0978760	-1.8097230	H	-2.0932770	5.7476490	-0.2829650
O	-6.1332590	1.0156850	-0.3419920	O	6.0860400	-0.0409630	-0.9366870
H	-6.6283560	0.4594500	0.2792120	H	6.1444960	0.1769710	-1.8800110
<p>TS Ylide S-3 (X=H, Y=OH) → <i>exo</i>-2-adduct (X=H, Y=OH)</p>  <p>E = -1279.38994891, H (0K) = -1279.043793, H (298K) = -1279.020701, G (298K) = -1279.095713 au.</p> <p>Imaginary frequency = 1.</p>				<p>Ylide U-3 (X=H, Y=OH)</p>  <p>E = -1279.41529444, H (0K) = -1279.069342, H (298K) = -1279.044854, G (298K) = -1279.124245 au.</p> <p>Imaginary frequency = 0.</p>			
C	-1.1801840	-2.4559570	-0.2222560	C	-1.1801840	-2.4559570	-0.2222560
C	-2.3808670	-1.7179100	-0.0201840	C	-2.3808670	-1.7179100	-0.0201840
C	0.1549180	-1.8941640	-0.3443420	C	0.1549180	-1.8941640	-0.3443420
O	-0.6901890	-0.1378570	-1.4955540	O	-0.6901890	-0.1378570	-1.4955540
C	-1.2091630	0.3595880	-0.4424210	C	-1.2091630	0.3595880	-0.4424210
O	-2.4508480	-0.3843420	0.0230250	O	-2.4508480	-0.3843420	0.0230250
N	0.7303750	-0.9497030	0.3977720	N	0.7303750	-0.9497030	0.3977720
C	-0.1767090	0.0247230	0.9490150	C	-0.1767090	0.0247230	0.9490150
C	0.4527460	1.2576620	1.5264690	C	0.4527460	1.2576620	1.5264690
O	1.3823410	1.8873350	1.0741870	O	1.3823410	1.8873350	1.0741870
O	-0.2284000	1.6487850	2.6347670	O	-0.2284000	1.6487850	2.6347670
H	0.8683990	-2.5057750	-0.8897450	H	0.8683990	-2.5057750	-0.8897450
H	-0.8245220	-0.4423010	1.6878550	H	-0.8245220	-0.4423010	1.6878550
H	0.1384380	2.5194000	2.8794890	H	0.1384380	2.5194000	2.8794890
C	-3.5940770	-2.4165590	0.1270330	C	-3.5940770	-2.4165590	0.1270330
C	-3.6356480	-3.7990780	0.0468520	C	-3.6356480	-3.7990780	0.0468520
H	-4.5870440	-4.3117570	0.1616520	H	-4.5870440	-4.3117570	0.1616520
C	-2.4683130	-4.5360340	-0.2081400	C	-2.4683130	-4.5360340	-0.2081400
C	-1.2687910	-3.8620400	-0.3544840	C	-1.2687910	-3.8620400	-0.3544840
H	-2.5046250	-5.6173850	-0.2948900	H	-2.5046250	-5.6173850	-0.2948900
H	-0.3568300	-4.4200760	-0.5545740	H	-0.3568300	-4.4200760	-0.5545740
H	-4.4943900	-1.8307580	0.2814930	H	-4.4943900	-1.8307580	0.2814930
C	2.1350820	-0.6847060	0.1508950	C	2.1350820	-0.6847060	0.1508950
C	3.0625030	-0.9318690	1.1640100	C	3.0625030	-0.9318690	1.1640100
C	2.5531430	-0.2297620	-1.0989720	C	2.5531430	-0.2297620	-1.0989720
C				C	4.4173460	-0.7236760	0.9313760

C	4.4173460	-0.7236760	0.9313760	H	2.7227680	-1.2904830	2.1312720
H	2.7227680	-1.2904830	2.1312720	C	3.9102280	-0.0268390	-1.3362240
C	3.9102280	-0.0268390	-1.3362240	H	1.8068980	-0.0193770	-1.8578100
H	1.8068980	-0.0193770	-1.8578100	C	4.8442460	-0.2690210	-0.3222190
C	4.8442460	-0.2690210	-0.3222190	H	5.1563420	-0.9103700	1.7035010
H	5.1563420	-0.9103700	1.7035010	H	4.2421550	0.3334100	-2.3080790
H	4.2421550	0.3334100	-2.3080790	C	-1.6165220	1.8237680	-0.4674330
C	-1.6165220	1.8237680	-0.4674330	C	-2.5208050	2.3625740	0.4556030
C	-2.5208050	2.3625740	0.4556030	C	-1.0582170	2.6527030	-1.4451130
C	-1.0582170	2.6527030	-1.4451130	C	-2.8607270	3.7147570	0.3973570
C	-2.8607270	3.7147570	0.3973570	H	-2.9667340	1.7214340	1.2081390
H	-2.9667340	1.7214340	1.2081390	C	-1.3943420	4.0052120	-1.4980650
C	-1.3943420	4.0052120	-1.4980650	H	-0.3717210	2.2186840	-2.1635460
H	-0.3717210	2.2186840	-2.1635460	C	-2.2968290	4.5406170	-0.5771940
C	-2.2968290	4.5406170	-0.5771940	H	-3.5714160	4.1218760	1.1123410
H	-3.5714160	4.1218760	1.1123410	H	-0.9553240	4.6399570	-2.2635550
H	-0.9553240	4.6399570	-2.2635550	H	-2.5629400	5.5937060	-0.6211420
H	-2.5629400	5.5937060	-0.6211420	O	6.1855050	-0.0850690	-0.4958700
O	6.1855050	-0.0850690	-0.4958700	H	6.3465250	0.2529820	-1.3906300
H	6.3465250	0.2529820	-1.3906300				
<p>TS Ylide U-3 (X=H, Y=OH) → <i>endo</i>-2-adduct (X=H, Y=OH)</p>  <p>E = -1279.39549771, H (0K) = -1279.049035, H (298K) = -1279.026083, G (298K) = -1279.101088 au.</p> <p>Imaginary frequency = 1.</p>							
C	-3.5041370	-3.5466240	-0.6176380				
C	-2.3395850	-4.2645880	-0.9283240				
C	-1.1222070	-3.6050640	-0.9209750				
C	-1.0210420	-2.2390740	-0.5744270				
C	-2.2142120	-1.5138930	-0.3121020				
C	-3.4446310	-2.1909500	-0.3303990				
C	0.3167040	-1.6817420	-0.5570210				
O	-2.2434710	-0.2004230	-0.0644740				
C	-0.9849460	0.5786840	-0.4652050				
O	-0.4641220	0.1622760	-1.5658700				
N	0.8807350	-0.8207110	0.2946680				
C	0.0395340	0.2383530	0.8198780				
C	-0.6529080	-0.1607830	2.1009290				
O	-0.7825430	-1.2901100	2.5184630				
O	-1.1141540	0.9276240	2.7616790				
H	-4.4681240	-4.0485890	-0.6231640				
H	-2.3904160	-5.3201120	-1.1762060				
H	-0.2112340	-4.1481300	-1.1623090				
H	-4.3418360	-1.6143680	-0.1301520				
H	1.0498780	-2.2549530	-1.1198470				
H	0.6584700	1.1169140	1.0025340				
H	-1.5789890	0.5848930	3.5482230				

C	2.2877480	-0.5336450	0.1317900
C	3.1544140	-0.7500270	1.2066960
C	2.7719020	-0.0307250	-1.0774770
C	4.5104620	-0.4729890	1.0728540
H	2.7614470	-1.1453780	2.1386480
C	4.1321410	0.2400770	-1.2156070
H	2.0717940	0.1622080	-1.8843530
C	5.0035410	0.0205010	-0.1422140
H	5.2020850	-0.6387490	1.8922530
H	4.5135620	0.6334830	-2.1559330
C	-1.4016730	2.0471770	-0.4301130
C	-2.4621740	2.5220140	0.3487870
C	-0.6757430	2.9476790	-1.2181420
C	-2.7859630	3.8799510	0.3404280
H	-3.0375360	1.8294560	0.9503070
C	-0.9944980	4.3051140	-1.2178440
H	0.1257580	2.5659170	-1.8416820
C	-2.0520850	4.7764270	-0.4373740
H	-3.6171600	4.2365450	0.9437050
H	-0.4235820	4.9933020	-1.8362470
H	-2.3060660	5.8333770	-0.4402230
O	6.3426040	0.2697800	-0.2158930
H	6.5564390	0.6107510	-1.0984710