

Supporting Information

Mechanistic Studies on the Electrocatalytic Reduction of CO₂ to Formate by Water-Stable Iridium Dihydride Pincer Complex

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Full Gaussian 09 Reference

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford, CT, 2009.

Theoretical Calculations.

All calculations were carried out using DFT as implemented in Gaussian 09. We chose to use the popular B3LYP functional, which includes Becke's three-parameter hybrid functional combined with the Lee–Yang–Parr correction for correlation. The standard 6-31G(d,p) basis set are used for H, C, N, O, and P atoms, while the effective core potentials (ECPs) of Hay and Wadt are combined with double- ζ valence basis sets (LanL2DZ) for Iridium. All structures studied in this paper were optimized. And all of the structures of transition states were presented in Figures. When necessary, IRC (intrinsic reaction coordinate) calculations were performed. Frequency calculations at the same level of theory have also been calculated to identify all stationary points as minima (zero imaginary frequencies) or first-order saddle points (one imaginary frequency) and to provide free energies at 298.15 K and 1 atm pressure, which include entropic contributions by considering the vibrations, rotations, and translations of the structures.

Solvent effects have also been taken into consideration. Single-point calculations with self-consistent reaction field based on the integral equation formalism polarizable continuum model (IEFPCM) with UAKS radii and cavity-dispersion-solvent-structure terms in Truhlar and co-workers' SMD solvation model for water and acetonitrile were applied for all gas-phase optimized structures at B3LYP/6-311++G(d,p) level. For all cited energies, ZPE corrections were taken into account. The electrons were given an energy of zero that corresponds to zero cell potential ($U=0V$). In order to evaluate the direction and magnitude of the donor–acceptor interactions for some stationary points, natural bond orbital (NBO) analysis was also performed. The Los Alamos National Laboratory 2-Double-Zeta (LANL2DZ) basis set was used for the Iridium atom, and the other atoms were computed with 6-311++G(d,p) basis.

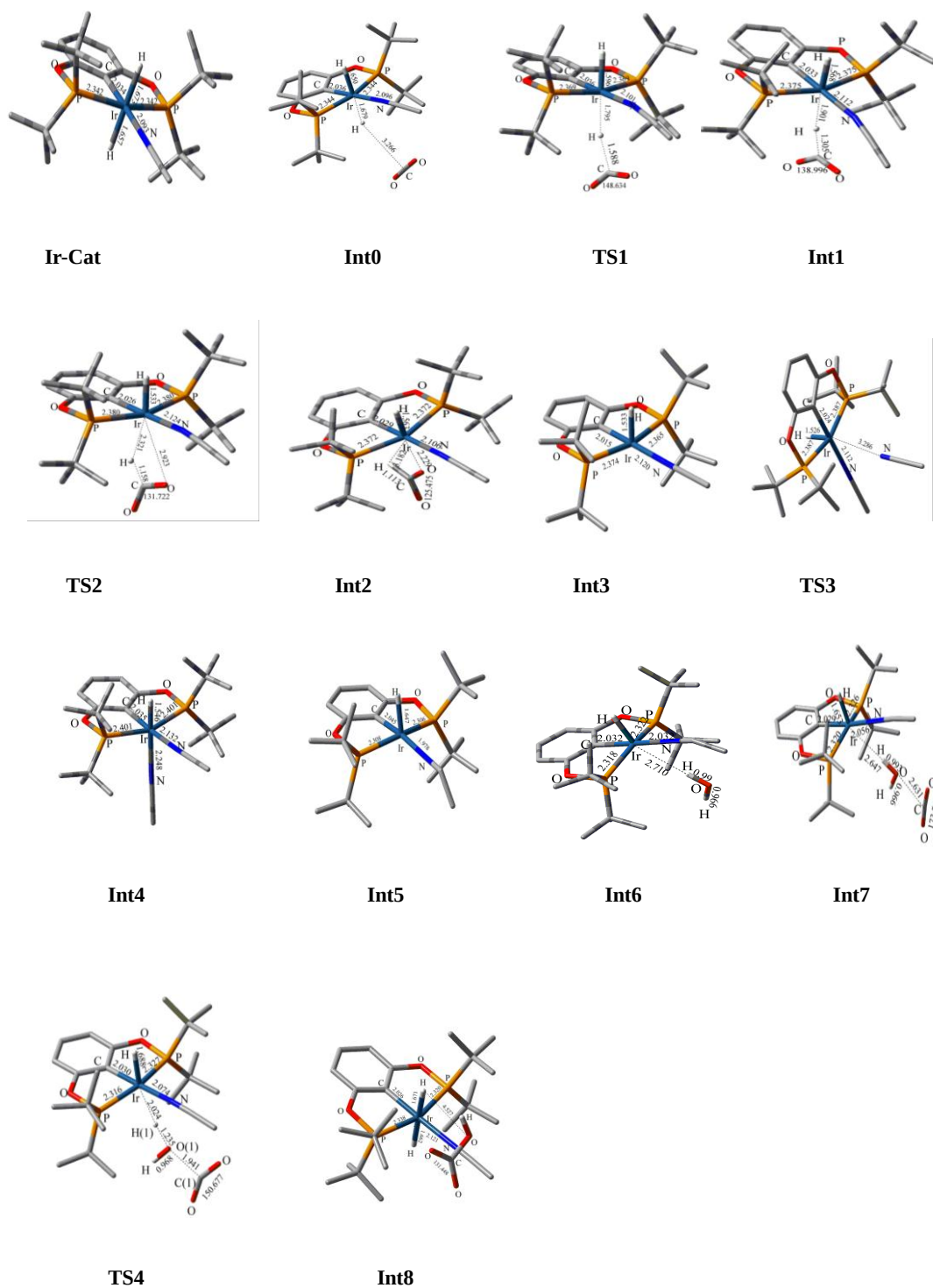
Table1: Calculated relative energies (all in kcal/mol, relative to Ir-Cat + 2CO₂ + H₂O + CNCH₃ + 2e⁻) for the ZPE-corrected Gibbs free energies (ΔG_{gas}), relative solvation energies (ΔG_{solv}) and Gibbs free energies (ΔG_{sol}) for all species in acetonitrile at 298 K by B3LYP/6-311++G(d,p)//B3LYP/6-31G(d,p) method.

species	ΔG_{gas}	ΔG_{solv}	ΔG_{sol}
Ir-Cat + 2CO ₂ + H ₂ O + CNCH ₃ + 2e ⁻	0.0	0.0	0.0
Int0 + H ₂ O + CNCH ₃ + 2e ⁻ + CO ₂	9.4	0.4	9.8
TS1 + CNCH ₃ + 2e ⁻ + CO ₂	22.7	-5.3	17.4
Int1 + H ₂ O + CNCH ₃ + 2e ⁻ + CO ₂	21.9	-6.6	15.3
TS2 + CNCH ₃ + 2e ⁻ + CO ₂	36.0	-16.1	19.9
Int2 + H ₂ O + CNCH ₃ + 2e ⁻ + CO ₂	16.8	-10.3	6.5
Int3 + HCOO ⁻ + CNCH ₃ + 2e ⁻ + H ₂ O + CO ₂	88.3	-102.1	-13.8
TS3 + HCOO ⁻ + 2e ⁻ + H ₂ O + CO ₂	97.1	-94.6	2.5
Int4 + HCOO ⁻ + 2e ⁻ + H ₂ O + CO ₂	84.2	-90.8	-6.6
Int5 + HCOO ⁻ + H ₂ O + CO ₂	-29.5	-104.7	-134.2
Int6 + HCOO ⁻ + CO ₂	-24.9	-96.6	-121.5
Int7 + HCOO ⁻	-20.3	-96.9	-117.2
TS4 + HCOO ⁻	-7.4	-98.3	-105.7
Int8 + HCOO ⁻	-52.4	-89.1	-141.5
Ir-Cat + HCO ₃ ⁻ + HCOO ⁻	-74.1	-117.8	-191.9

Table2: Calculated relative energies (all in kcal/mol, relative to Ir-Cat + 2CO₂ + H₂O + CNCH₃ + 2e⁻) for the ZPE-corrected Gibbs free energies (ΔG_{gas}), relative solvation energies (ΔG_{solv}) and Gibbs free energies (ΔG_{sol}) for all species in water at 298 K by B3LYP/6-311++G(d,p)//B3LYP/6-31G(d,p) method.

species	ΔG_{gas}	ΔG_{solv}	ΔG_{sol}
Ir-Cat + 2CO ₂ + H ₂ O + CNCH ₃ + 2e ⁻	0.0	0.0	0.0
Int0 + H ₂ O + CNCH ₃ + 2e ⁻ + CO ₂	9.4	-1.4	8.0
TS1 + CNCH ₃ + 2e ⁻ + CO ₂	22.7	-8.3	14.4
Int1 + H ₂ O + CNCH ₃ + 2e ⁻ + CO ₂	21.9	-9.7	12.2
TS2 + CNCH ₃ + 2e ⁻ + CO ₂	36.0	-19.3	16.7
Int2 + H ₂ O + CNCH ₃ + 2e ⁻ + CO ₂	16.8	-13.4	3.4
Int3 + HCOO ⁻ + CNCH ₃ + 2e ⁻ + H ₂ O + CO ₂	88.3	-107.4	-19.1
TS3 + HCOO ⁻ + 2e ⁻ + H ₂ O + CO ₂	97.1	-99.9	-2.8
Int4 + HCOO ⁻ + 2e ⁻ + H ₂ O + CO ₂	84.2	-96.9	-12.7
Int5 + HCOO ⁻ + H ₂ O + CO ₂	-29.5	-110.3	-139.8
Int6 + HCOO ⁻ + CO ₂	-24.9	-103.7	-128.6
Int7 + HCOO ⁻	-20.3	-104.8	-125.1
TS4 + HCOO ⁻	-7.4	-106.4	-113.8
Int8 + HCOO ⁻	-52.4	-114.1	-166.5
Ir-Cat + HCO ₃ ⁻ + HCOO ⁻	-74.1	-137.7	-211.8

Figure 1. Optimized structures and selected geometric parameters of species.



Optimized Cartesian coordinates (in Å)

Optimized Cartesian coordinates for Ir-Cat.

Ir	0.00000200	-0.31594600	-0.04809900
P	2.30249400	0.10920600	-0.00964700
P	-2.30249500	0.10921900	-0.00960900
O	2.40053200	1.77766200	-0.13161400
C	1.18442700	2.46093700	-0.13618200
C	1.21324800	3.85410100	-0.18329700
H	2.16443900	4.37573700	-0.20450700
C	0.00002400	4.54628000	-0.20520100
H	0.00002700	5.63165200	-0.24131400
C	-1.21320500	3.85411400	-0.18314600
H	-2.16439300	4.37576000	-0.20424100
C	-1.18439500	2.46094900	-0.13603100
C	0.00001500	1.71716100	-0.10334500
O	-2.40051200	1.77769600	-0.13129800
C	3.19024600	-0.20365500	1.65832000
C	2.57058600	0.78008200	2.67549500
H	1.48321700	0.69056400	2.70988900
H	2.82869900	1.81466800	2.43581600
H	2.96904800	0.55032000	3.67129700
C	4.71198400	0.02840100	1.64930900
H	5.08391200	-0.05999100	2.67756100
H	4.97029600	1.02854800	1.29171000
H	5.24973600	-0.71049000	1.04983200
C	2.88706100	-1.64936700	2.10327100
H	3.32557200	-2.39280100	1.42918700
H	1.80946600	-1.82127700	2.16057400
H	3.31711800	-1.81712000	3.09849100
C	3.41812000	-0.36948300	-1.48719000
C	4.70137400	0.48491700	-1.57631400
H	5.43596300	0.24232000	-0.80965000
H	4.46932200	1.55053700	-1.51066100
H	5.17531300	0.30351900	-2.54866100
C	3.76266700	-1.86886600	-1.40979700
H	4.28777600	-2.16919100	-2.32468500
H	2.86023200	-2.48397100	-1.33095600
H	4.41688700	-2.10515100	-0.56550200
C	2.60770400	-0.10699900	-2.77496600
H	3.24075900	-0.34413500	-3.63904100
H	2.30877700	0.94237400	-2.85190100
H	1.70085900	-0.71041400	-2.81930500
C	-3.19029100	-0.20386700	1.65830000
C	-2.57066700	0.77976900	2.67559300

H	-2.96911300	0.54986700	3.67137000
H	-2.82881900	1.81437300	2.43603800
H	-1.48329400	0.69028500	2.70996800
C	-2.88705500	-1.64961600	2.10308200
H	-1.80946200	-1.82153500	2.16032100
H	-3.32559000	-2.39297900	1.42893300
H	-3.31707500	-1.81750100	3.09829300
C	-4.71203700	0.02812200	1.64931800
H	-5.24975700	-0.71076000	1.04979900
H	-4.97041300	1.02827700	1.29178900
H	-5.08394500	-0.06036400	2.67756900
C	-3.41807200	-0.36923700	-1.48727700
C	-3.76238000	-1.86869300	-1.41029800
H	-4.28760900	-2.16881600	-2.32518200
H	-4.41640800	-2.10533300	-0.56595000
H	-2.85981800	-2.48366800	-1.33185500
C	-4.70146800	0.48498000	-1.57614000
H	-4.46960400	1.55061500	-1.51004800
H	-5.43606600	0.24194600	-0.80962500
H	-5.17531300	0.30389500	-2.54859100
C	-2.60773500	-0.10625300	-2.77499800
H	-1.70079000	-0.70950200	-2.81954000
H	-2.30899700	0.94319500	-2.85163900
H	-3.24077500	-0.34324800	-3.63912300
N	-0.00002400	-2.40892500	-0.06057400
C	-0.00004000	-3.56840500	-0.07778700
C	-0.00005600	-5.02647700	-0.09872000
H	0.04475800	-5.39326700	-1.12867000
H	0.86464000	-5.41311800	0.44893500
H	-0.91002900	-5.41172100	0.37099000
H	-0.00002200	-0.31620800	-1.70516400
H	0.00002500	-0.32818200	1.62527200

Optimized Cartesian coordinates for Int0.

Ir	0.00000600	-0.01909400	0.33709600
P	2.30455000	-0.38319200	0.11311800
P	-2.30454500	-0.38317100	0.11315200
O	2.39995300	-1.84506800	-0.69911500
C	1.18372700	-2.42367000	-1.06085100
C	1.21289100	-3.62885700	-1.76143300
H	2.16437800	-4.08200500	-2.01946500
C	-0.00002800	-4.22676600	-2.11137200
H	-0.00003700	-5.16528900	-2.65769700
C	-1.21293700	-3.62887600	-1.76136300

H	-2.16443100	-4.08204000	-2.01933900
C	-1.18375200	-2.42368800	-1.06078300
C	-0.00000700	-1.77475400	-0.69388200
O	-2.39996500	-1.84511100	-0.69896800
C	3.24029400	0.77332900	-1.09300000
C	2.61673100	0.54622000	-2.48809900
H	1.53521900	0.69436200	-2.47559800
H	2.82611500	-0.46116800	-2.85654300
H	3.05825600	1.26437700	-3.18997300
C	4.75486100	0.52016400	-1.20911800
H	5.15366800	1.15086200	-2.01338600
H	4.97621900	-0.51894700	-1.46667700
H	5.29838800	0.78126500	-0.29759300
C	2.99213900	2.23121600	-0.65651000
H	3.46329500	2.46528900	0.30342600
H	1.92353900	2.44001400	-0.57273500
H	3.42247900	2.90924600	-1.40417200
C	3.38370800	-0.80879200	1.63548100
C	4.65940100	-1.59763800	1.26634400
H	5.40558300	-0.99519600	0.75060400
H	4.42169600	-2.46278400	0.64285700
H	5.12091400	-1.96559500	2.19062200
C	3.74171000	0.48142000	2.39713400
H	4.24681500	0.22051400	3.33506900
H	2.84671300	1.05782500	2.65467600
H	4.41901100	1.12703200	1.83096300
C	2.54165800	-1.71555200	2.55842800
H	3.16301800	-2.01740200	3.41069400
H	2.21370600	-2.62141800	2.04044900
H	1.65188200	-1.20674300	2.92912400
C	-3.24027700	0.77324700	-1.09307400
C	-2.61664400	0.54606800	-2.48813000
H	-3.05817100	1.26415600	-3.19007400
H	-2.82596700	-0.46135500	-2.85651500
H	-1.53513900	0.69425900	-2.47559300
C	-2.99220800	2.23117700	-0.65667500
H	-1.92362600	2.44002300	-0.57278100
H	-3.46349000	2.46532100	0.30318100
H	-3.42247200	2.90913300	-1.40444600
C	-4.75482700	0.51999600	-1.20923400
H	-5.29839800	0.78108000	-0.29773000
H	-4.97611600	-0.51913300	-1.46678300
H	-5.15364700	1.15065600	-2.01352700
C	-3.38373400	-0.80864700	1.63552600

C	-3.74189900	0.48163800	2.39697900
H	-4.24696900	0.22080700	3.33495400
H	-4.41928400	1.12708000	1.83071400
H	-2.84697600	1.05819600	2.65443400
C	-4.65933900	-1.59764900	1.26643300
H	-4.42152000	-2.46289900	0.64313300
H	-5.40551400	-0.99535700	0.75050800
H	-5.12090700	-1.96545700	2.19074200
C	-2.54166300	-1.71520100	2.55865600
H	-1.65198200	-1.20623900	2.92937000
H	-2.21355100	-2.62109300	2.04082400
H	-3.16306300	-2.01701600	3.41090400
N	0.00002900	1.78763500	1.39876800
C	0.00003400	2.82172200	1.92245300
C	0.00007600	4.14712600	2.52896900
H	0.88853700	4.28160200	3.15291700
H	-0.00005100	4.90694100	1.74173200
H	-0.88822000	4.28155500	3.15316400
H	0.00000900	-0.88170200	1.74417300
H	0.00000800	0.88083400	-1.08039500
C	-0.00000200	3.97984100	-2.11263300
O	0.00000600	3.51942300	-3.18530600
O	-0.00001300	4.46703600	-1.04679700

Optimized Cartesian coordinates for TS1.

Ir	-0.29816513	2.52293574	0.00000000
P	2.02904287	2.08848874	-0.07848100
P	-2.62537913	2.08850474	-0.07849800
O	2.10066287	0.53632374	-0.70166200
C	0.88604487	-0.05915626	-1.03197600
C	0.91462787	-1.35265626	-1.55166900
H	1.86574587	-1.84441526	-1.72591000
C	-0.29817113	-1.98996126	-1.82124700
H	-0.29817313	-2.99624126	-2.22926300
C	-1.51096813	-1.35263826	-1.55170100
H	-2.46208913	-1.84438326	-1.72596600
C	-1.48238013	-0.05913826	-1.03200700
C	-0.29816513	0.64919074	-0.79573400
O	-2.69700013	0.53635574	-0.70172000
C	3.11261687	3.01204374	-1.34905600
C	2.56351687	2.61341474	-2.73860600
H	1.48771987	2.75548174	-2.83435200
H	2.79376187	1.56881574	-2.96141700
H	3.04936587	3.23882274	-3.49684800

C	4.60671487	2.63694074	-1.32249800
H	5.09273987	3.10673174	-2.18621900
H	4.75973487	1.55800074	-1.40633000
H	5.12047287	3.00111574	-0.42920500
C	2.96738887	4.53211574	-1.13086700
H	3.40327287	4.85352674	-0.17977900
H	1.92811487	4.86126474	-1.16168800
H	3.50691587	5.05709574	-1.92826300
C	2.96582787	1.82896474	1.57153000
C	4.19062987	0.90073574	1.41390200
H	5.00190587	1.34948674	0.84315900
H	3.91211387	-0.04115426	0.93561300
H	4.58283987	0.67008674	2.41160700
C	3.38340987	3.19444774	2.14953200
H	3.77947187	3.05318274	3.16223200
H	2.53124987	3.87873274	2.22164000
H	4.16521087	3.67712774	1.55756000
C	2.00535387	1.14382874	2.56766900
H	2.56712887	0.89569474	3.47632800
H	1.59040687	0.21627174	2.16299300
H	1.17261487	1.79178174	2.84375400
C	-3.70895713	3.01210574	-1.34904000
C	-3.15989613	2.61348474	-2.73860600
H	-3.64578813	3.23887474	-3.49683500
H	-3.39011513	1.56887874	-2.96140600
H	-2.08410513	2.75558074	-2.83438300
C	-3.56367013	4.53216874	-1.13082700
H	-2.52438613	4.86128074	-1.16166100
H	-3.99952713	4.85357774	-0.17972600
H	-4.10319213	5.05718274	-1.92820400
C	-5.20306713	2.63705974	-1.32246600
H	-5.71677913	3.00115174	-0.42911400
H	-5.35613313	1.55813474	-1.40641800
H	-5.68910513	3.10696874	-2.18611600
C	-3.56216613	1.82893674	1.57150500
C	-3.97983013	3.19439374	2.14951000
H	-4.37589113	3.05309574	3.16220700
H	-4.76165513	3.67703774	1.55754000
H	-3.12771213	3.87872874	2.22163500
C	-4.78691313	0.90064074	1.41386100
H	-4.50828913	-0.04131626	0.93576800
H	-5.59813013	1.34925474	0.84292800
H	-5.17924813	0.67014774	2.41155400
C	-2.60167513	1.14384674	2.56765800

H	-1.76900013	1.79185774	2.84379800
H	-2.18663613	0.21633774	2.16296700
H	-3.16346713	0.89563474	3.47628600
N	-0.29817013	4.44990674	0.83837300
C	-0.29812213	5.58603674	1.05761000
C	-0.29810613	7.03310274	1.21062300
H	0.59164187	7.36575774	1.75242300
H	-0.29802913	7.47237474	0.20794400
H	-1.18791313	7.36578974	1.75230700
H	-0.29817813	1.77547974	1.41040500
H	-0.29812713	3.45779274	-1.53237800
C	-0.29811513	4.68690174	-2.53727000
O	-0.29806113	4.17860274	-3.62150600
O	-0.29816613	5.69094874	-1.87228300

Optimized Cartesian coordinates for Int1.

Ir	0.00000100	0.14921500	0.25730700
P	2.33473800	-0.27609300	0.16147300
P	-2.33471800	-0.27615500	0.16149200
O	2.39999400	-1.81724000	-0.48946300
C	1.18591100	-2.40133600	-0.83856300
C	1.21349000	-3.68137100	-1.39038000
H	2.16396100	-4.16964200	-1.57675900
C	0.00005200	-4.31044700	-1.67557700
H	0.00006400	-5.30608100	-2.10881900
C	-1.21339900	-3.68141400	-1.39034500
H	-2.16385800	-4.16971800	-1.57669600
C	-1.18584900	-2.40137800	-0.83852900
C	0.00002200	-1.69948000	-0.58799400
O	-2.39994200	-1.81732300	-0.48939300
C	3.41843000	0.67031100	-1.08939200
C	2.87975800	0.29438100	-2.48995600
H	1.81078400	0.46710900	-2.61314900
H	3.09244300	-0.75254300	-2.71935200
H	3.39352500	0.91623100	-3.23235800
C	4.91053500	0.28652900	-1.05451500
H	5.40541500	0.76861100	-1.90603200
H	5.05932100	-0.79156600	-1.15565500
H	5.41817200	0.63355500	-0.15096700
C	3.27794300	2.18781200	-0.84789900
H	3.69432400	2.49002100	0.11821600
H	2.24431900	2.53227000	-0.90413300
H	3.84259700	2.71826200	-1.62371600
C	3.25424600	-0.56645100	1.81369200

C	4.47225600	-1.50277700	1.65291300
H	5.28921500	-1.05412900	1.09016300
H	4.18951100	-2.43795400	1.16410000
H	4.85762700	-1.74561000	2.65031100
C	3.67804500	0.78742300	2.41438800
H	4.06719000	0.62725900	3.42686400
H	2.83106600	1.47734900	2.49213200
H	4.46664100	1.27269500	1.83408800
C	2.27747600	-1.25618000	2.79123100
H	2.82760600	-1.52415900	3.70115300
H	1.85614700	-2.17372700	2.37035800
H	1.45190900	-0.60091100	3.07378600
C	-3.41840300	0.67021000	-1.08941200
C	-2.87979400	0.29413700	-2.48996200
H	-3.39355900	0.91594900	-3.23239900
H	-3.09253700	-0.75279600	-2.71926200
H	-1.81081700	0.46681500	-2.61320600
C	-3.27781500	2.18772300	-0.84804500
H	-2.24416600	2.53210400	-0.90429400
H	-3.69418100	2.49004200	0.11804200
H	-3.84242500	2.71814700	-1.62391200
C	-4.91053300	0.28653400	-1.05446600
H	-5.41813500	0.63371000	-0.15095600
H	-5.05939400	-0.79156300	-1.15546800
H	-5.40539300	0.76854200	-1.90603800
C	-3.25421100	-0.56649100	1.81372100
C	-3.67824200	0.78737500	2.41427100
H	-4.06736700	0.62725200	3.42676200
H	-4.46691400	1.27245400	1.83391400
H	-2.83137800	1.47745000	2.49194900
C	-4.47205700	-1.50304500	1.65303400
H	-4.18915000	-2.43821200	1.16429500
H	-5.28910500	-1.05459100	1.09026000
H	-4.85737000	-1.74586600	2.65045800
C	-2.27733500	-1.25595400	2.79134300
H	-1.45189200	-0.60051000	3.07385300
H	-1.85583300	-2.17346400	2.37056200
H	-2.82743500	-1.52394900	3.70127900
N	-0.00004400	2.07558800	1.12340900
C	-0.00011600	3.22764100	1.23153500
C	-0.00021200	4.68110800	1.26183700
H	0.89065800	5.05939100	1.77062200
H	-0.00045600	5.01120200	0.21797900
H	-0.89091100	5.05927500	1.77101900

H	0.00001100	-0.64011700	1.61240200
H	-0.00002200	1.24669800	-1.29431000
C	-0.00004100	2.23669200	-2.14412300
O	-0.00030200	1.80036200	-3.28195700
O	0.00009900	3.32175800	-1.56680500

Optimized Cartesian coordinates for TS2.

Ir	-2.36238526	2.61467886	0.00000000
P	-0.02209026	3.04991986	0.01225600
P	-4.70270126	3.04969986	0.01224900
O	0.04296674	4.64207986	0.52994800
C	-1.17374326	5.26566186	0.79511400
C	-1.14782126	6.59674686	1.20840300
H	-0.19826326	7.10138686	1.34984800
C	-2.36259326	7.25125886	1.42323200
H	-2.36264326	8.28676086	1.74983400
C	-3.57730226	6.59662786	1.20840500
H	-4.52690826	7.10117586	1.34985100
C	-3.55125126	5.26554486	0.79511600
C	-2.36246226	4.54627286	0.61144200
O	-4.76790026	4.64184786	0.52995900
C	1.13000674	2.17844986	1.26544200
C	0.79821074	2.73930886	2.66742000
H	-0.23878026	2.60084486	2.96787600
H	1.04177074	3.80239886	2.73543400
H	1.41402574	2.20198186	3.39793900
C	2.63542674	2.41491486	1.03274500
H	3.17948474	1.93167686	1.85276600
H	2.89637774	3.47626686	1.05055200
H	3.00179774	1.97254386	0.10343300
C	0.83061574	0.66463586	1.21177700
H	1.07349974	0.23432186	0.23350800
H	-0.21362626	0.44728586	1.45282700
H	1.46236674	0.15978186	1.95241900
C	0.80227374	3.22180286	-1.70633300
C	2.05862574	4.12014986	-1.66934200
H	2.89859474	3.66527086	-1.14851100
H	1.83978074	5.08254786	-1.20013300
H	2.37941674	4.31228986	-2.69993000
C	1.13293174	1.82357286	-2.26259500
H	1.49606474	1.92106886	-3.29274800
H	0.24607074	1.18105286	-2.28433000
H	1.91118674	1.31568086	-1.68779200
C	-0.20805426	3.90331586	-2.65694200

H	0.30202274	4.13662186	-3.59889000
H	-0.59714526	4.83923286	-2.24577500
H	-1.05192926	3.25120086	-2.88905000
C	-5.85473926	2.17810186	1.26540300
C	-5.52295226	2.73886386	2.66742100
H	-6.13893226	2.20165386	3.39788600
H	-5.76623126	3.80201286	2.73548400
H	-4.48600926	2.60003286	2.96783500
C	-5.55521226	0.66430586	1.21170000
H	-4.51101326	0.44703186	1.45305400
H	-5.79776026	0.23401886	0.23333900
H	-6.18713726	0.15934886	1.95212500
C	-7.36016626	2.41449086	1.03269100
H	-7.72649826	1.97216086	0.10334400
H	-7.62117526	3.47582886	1.05055700
H	-7.90421426	1.93117286	1.85267000
C	-5.52707926	3.22152786	-1.70634200
C	-5.85766826	1.82328086	-2.26260700
H	-6.22079926	1.92076586	-3.29276300
H	-6.63590326	1.31534886	-1.68781300
H	-4.97078026	1.18079686	-2.28434300
C	-6.78347726	4.11981186	-1.66934700
H	-6.56468126	5.08221786	-1.20013400
H	-7.62342326	3.66488886	-1.14852000
H	-7.10427526	4.31193986	-2.69993500
C	-4.51679426	3.90308986	-2.65696100
H	-3.67287226	3.25103086	-2.88905200
H	-4.12777226	4.83904386	-2.24581200
H	-5.02688526	4.13633886	-3.59891600
N	-2.36228326	0.60412586	-0.68396800
C	-2.36184326	-0.53673914	-0.86989200
C	-2.36134126	-1.98813514	-0.98599800
H	-3.25096526	-2.33204414	-1.52081600
H	-1.47134326	-2.33143414	-1.52058700
H	-2.36131726	-2.41594014	0.02138200
H	-2.36239326	3.16378286	-1.43147000
H	-2.36249626	2.55100686	2.32018800
C	-2.36228426	1.52508786	2.85672400
O	-2.36228226	1.58382786	4.08490000
O	-2.36212226	0.54018786	2.05963700

Optimized Cartesian coordinates for Int2.

Ir	-0.16949152	1.46610166	0.00000000
P	2.17744948	1.07988266	-0.20065800

P	-2.51643052	1.07965466	-0.20047000
O	2.23571748	-0.20238834	-1.27089800
C	1.02122448	-0.67005434	-1.75991800
C	1.04656748	-1.72791534	-2.66544800
H	1.99443248	-2.14059234	-2.99215300
C	-0.16943252	-2.24348034	-3.11923700
H	-0.16942052	-3.06844434	-3.82448700
C	-1.38544652	-1.72803034	-2.66535500
H	-2.33329752	-2.14079834	-2.99198900
C	-1.36013752	-0.67016634	-1.75982700
C	-0.16946752	-0.07785234	-1.30825400
O	-2.57463852	-0.20261334	-1.27072100
C	3.20284448	2.37418066	-1.13781000
C	2.58531748	2.44093166	-2.55382100
H	1.50967948	2.62703966	-2.53252600
H	2.76817948	1.51937566	-3.11055000
H	3.05605048	3.26624266	-3.10019700
C	4.69345948	2.01352566	-1.28179000
H	5.15612648	2.72830366	-1.97225800
H	4.83582648	1.01378666	-1.69946800
H	5.23671148	2.08430766	-0.33638500
C	3.05896148	3.74078166	-0.43643000
H	3.49101648	3.73987766	0.56797800
H	2.01541548	4.05612766	-0.37072500
H	3.60094848	4.49364466	-1.02061100
C	3.08936248	0.33450966	1.29460700
C	4.31009948	-0.50567934	0.86021400
H	5.10924348	0.09493966	0.42787800
H	4.02837648	-1.27664034	0.13996300
H	4.71789448	-1.00353634	1.74688700
C	3.51658148	1.45257966	2.26495000
H	3.91928248	0.99766366	3.17669800
H	2.67268348	2.08530666	2.56082500
H	4.30003748	2.08958166	1.84672100
C	2.10122548	-0.61002134	2.01483900
H	2.64062248	-1.14595934	2.80350200
H	1.67719048	-1.35661034	1.33703300
H	1.28239748	-0.06184434	2.48780100
C	-3.54207452	2.37379566	-1.13756000
C	-2.92458252	2.44067266	-2.55357900
H	-3.39544652	3.26592366	-3.09993400
H	-3.10731852	1.51910366	-3.11032800
H	-1.84897652	2.62693166	-2.53229100
C	-3.39845952	3.74040666	-0.43614300

H	-2.35498652	4.05595166	-0.37031300
H	-3.83061852	3.73940066	0.56822300
H	-3.94053652	4.49319566	-1.02033800
C	-5.03262652	2.01287066	-1.28153600
H	-5.57588752	2.08357666	-0.33613000
H	-5.17481552	1.01309566	-1.69919000
H	-5.49542252	2.72755066	-1.97201800
C	-3.42813852	0.33419866	1.29488300
C	-3.85537552	1.45223766	2.26525100
H	-4.25800052	0.99729466	3.17701800
H	-4.63889752	2.08918366	1.84705600
H	-3.01149452	2.08500166	2.56110500
C	-4.64883452	-0.50611134	0.86060800
H	-4.36710452	-1.27705434	0.14033800
H	-5.44807952	0.09442266	0.42833900
H	-5.05649952	-1.00400134	1.74732200
C	-2.43984452	-0.61022534	2.01503600
H	-1.62102752	-0.06195734	2.48790900
H	-2.01580752	-1.35679034	1.33720500
H	-2.97911652	-1.14619534	2.80376400
N	-0.16950652	3.06971466	1.37445900
C	-0.16948652	3.93756766	2.14199500
C	-0.16927052	5.03138766	3.10533800
H	0.70090048	5.67409066	2.94379100
H	-1.07777752	5.63027466	2.99443800
H	-0.13047752	4.63412366	4.12385900
H	-0.16939352	0.42322666	1.11402000
N	-0.16968252	4.28307866	-1.69170400
C	-0.17015152	5.21946266	-2.37763600
C	-0.17084052	6.39017366	-3.24925200
H	0.71526748	7.00211866	-3.05963200
H	-0.16452352	6.07495966	-4.29640400
H	-1.06380652	6.99468166	-3.06813400

Optimized Cartesian coordinates for Int3.

Ir	-0.01070200	-0.29851100	-0.04611400
P	2.33108900	0.09402000	-0.03746000
P	-2.33654000	0.12997000	-0.03012800
O	2.41021600	1.76205600	-0.13809100
C	1.20389900	2.44853800	-0.08246900
C	1.23900200	3.84008300	-0.06444400
H	2.18947300	4.36113100	-0.08532000
C	0.02727400	4.53445200	-0.02491200
H	0.03624500	5.61963100	-0.01249900

C	-1.19586100	3.85950900	-0.00262500
H	-2.13776600	4.39556800	0.02457600
C	-1.18334800	2.46776700	-0.02105400
C	0.00449500	1.71607300	-0.04842600
O	-2.40261700	1.79972500	-0.00902900
C	3.14626300	-0.23163900	1.64415300
C	2.32981400	0.59018400	2.66838200
H	1.27097200	0.30826700	2.67925200
H	2.39462300	1.66390900	2.47925800
H	2.72871700	0.39879000	3.67049200
C	4.61810400	0.21498400	1.70872200
H	4.96218300	0.14582900	2.74691100
H	4.74537800	1.25135900	1.38573600
H	5.27061200	-0.42408600	1.10921300
C	3.02582900	-1.72832700	1.99817800
H	3.58659400	-2.37035300	1.31501100
H	1.98345700	-2.06091500	2.00671500
H	3.43284900	-1.88668000	3.00303600
C	3.39672800	-0.38520000	-1.53155200
C	4.63527900	0.52636700	-1.66607800
H	5.35202100	0.39279900	-0.85565400
H	4.35480900	1.58056500	-1.70902100
H	5.14773500	0.27442700	-2.60121100
C	3.82039400	-1.86344000	-1.43744400
H	4.29434200	-2.15601100	-2.38076200
H	2.96513000	-2.52969100	-1.28152800
H	4.54930700	-2.03805000	-0.64180000
C	2.51447200	-0.18710400	-2.78520800
H	3.12913600	-0.35578300	-3.67602100
H	2.11217800	0.82819200	-2.84824000
H	1.68164100	-0.89505900	-2.81579700
C	-3.15542900	-0.28737500	1.62536500
C	-2.06120600	-0.01475500	2.68568700
H	-2.46602000	-0.21990000	3.68319300
H	-1.72527100	1.02602400	2.67178700
H	-1.18935300	-0.66880200	2.55080900
C	-3.54481300	-1.77718000	1.67136400
H	-2.70247400	-2.43179400	1.42313300
H	-4.37557900	-2.00947500	1.00032600
H	-3.86816200	-2.02871000	2.68755100
C	-4.37326400	0.60444600	1.93843400
H	-5.22427000	0.39854500	1.28805500
H	-4.12546500	1.66500900	1.85778900
H	-4.69322200	0.40884700	2.96822900

C	-3.36266800	-0.28306600	-1.56250200
C	-3.20316100	-1.78328000	-1.88397100
H	-3.73714500	-2.00309400	-2.81485400
H	-3.62444200	-2.42702300	-1.10722700
H	-2.15329500	-2.05452300	-2.02829000
C	-4.85148600	0.07814600	-1.39899300
H	-4.98814000	1.12182200	-1.10373900
H	-5.35815400	-0.56301800	-0.67361500
H	-5.35477600	-0.06129400	-2.36221500
C	-2.77169900	0.55232300	-2.72090100
H	-1.70962100	0.34650300	-2.88198700
H	-2.89258700	1.62420400	-2.54999800
H	-3.30421700	0.29299200	-3.64223100
N	-0.03805200	-2.41735400	0.01351000
C	-0.05367300	-3.57649500	0.02581000
C	-0.07321300	-5.03376400	0.03650000
H	0.70083900	-5.41509600	0.70876600
H	-1.04784100	-5.39499400	0.37702900
H	0.11327300	-5.41635600	-0.97134300
H	-0.00272800	-0.32848000	-1.57859600

Optimized Cartesian coordinates for TS3.

Ir	-0.16949152	1.46610166	0.00000000
P	2.17744948	1.07988266	-0.20065800
P	-2.51643052	1.07965466	-0.20047000
O	2.23571748	-0.20238834	-1.27089800
C	1.02122448	-0.67005434	-1.75991800
C	1.04656748	-1.72791534	-2.66544800
H	1.99443248	-2.14059234	-2.99215300
C	-0.16943252	-2.24348034	-3.11923700
H	-0.16942052	-3.06844434	-3.82448700
C	-1.38544652	-1.72803034	-2.66535500
H	-2.33329752	-2.14079834	-2.99198900
C	-1.36013752	-0.67016634	-1.75982700
C	-0.16946752	-0.07785234	-1.30825400
O	-2.57463852	-0.20261334	-1.27072100
C	3.20284448	2.37418066	-1.13781000
C	2.58531748	2.44093166	-2.55382100
H	1.50967948	2.62703966	-2.53252600
H	2.76817948	1.51937566	-3.11055000
H	3.05605048	3.26624266	-3.10019700
C	4.69345948	2.01352566	-1.28179000
H	5.15612648	2.72830366	-1.97225800
H	4.83582648	1.01378666	-1.69946800

H	5.23671148	2.08430766	-0.33638500
C	3.05896148	3.74078166	-0.43643000
H	3.49101648	3.73987766	0.56797800
H	2.01541548	4.05612766	-0.37072500
H	3.60094848	4.49364466	-1.02061100
C	3.08936248	0.33450966	1.29460700
C	4.31009948	-0.50567934	0.86021400
H	5.10924348	0.09493966	0.42787800
H	4.02837648	-1.27664034	0.13996300
H	4.71789448	-1.00353634	1.74688700
C	3.51658148	1.45257966	2.26495000
H	3.91928248	0.99766366	3.17669800
H	2.67268348	2.08530666	2.56082500
H	4.30003748	2.08958166	1.84672100
C	2.10122548	-0.61002134	2.01483900
H	2.64062248	-1.14595934	2.80350200
H	1.67719048	-1.35661034	1.33703300
H	1.28239748	-0.06184434	2.48780100
C	-3.54207452	2.37379566	-1.13756000
C	-2.92458252	2.44067266	-2.55357900
H	-3.39544652	3.26592366	-3.09993400
H	-3.10731852	1.51910366	-3.11032800
H	-1.84897652	2.62693166	-2.53229100
C	-3.39845952	3.74040666	-0.43614300
H	-2.35498652	4.05595166	-0.37031300
H	-3.83061852	3.73940066	0.56822300
H	-3.94053652	4.49319566	-1.02033800
C	-5.03262652	2.01287066	-1.28153600
H	-5.57588752	2.08357666	-0.33613000
H	-5.17481552	1.01309566	-1.69919000
H	-5.49542252	2.72755066	-1.97201800
C	-3.42813852	0.33419866	1.29488300
C	-3.85537552	1.45223766	2.26525100
H	-4.25800052	0.99729466	3.17701800
H	-4.63889752	2.08918366	1.84705600
H	-3.01149452	2.08500166	2.56110500
C	-4.64883452	-0.50611134	0.86060800
H	-4.36710452	-1.27705434	0.14033800
H	-5.44807952	0.09442266	0.42833900
H	-5.05649952	-1.00400134	1.74732200
C	-2.43984452	-0.61022534	2.01503600
H	-1.62102752	-0.06195734	2.48790900
H	-2.01580752	-1.35679034	1.33720500
H	-2.97911652	-1.14619534	2.80376400

N	-0.16950652	3.06971466	1.37445900
C	-0.16948652	3.93756766	2.14199500
C	-0.16927052	5.03138766	3.10533800
H	0.70090048	5.67409066	2.94379100
H	-1.07777752	5.63027466	2.99443800
H	-0.13047752	4.63412366	4.12385900
H	-0.16939352	0.42322666	1.11402000
N	-0.16968252	4.28307866	-1.69170400
C	-0.17015152	5.21946266	-2.37763600
C	-0.17084052	6.39017366	-3.24925200
H	0.71526748	7.00211866	-3.05963200
H	-0.16452352	6.07495966	-4.29640400
H	-1.06380652	6.99468166	-3.06813400

Optimized Cartesian coordinates for Int4.

Ir	-0.00000900	-0.24305700	-0.11976000
P	2.35258900	0.23393400	-0.18028200
P	-2.35263600	0.23368000	-0.18070800
O	2.40464400	1.80579800	0.37270400
C	1.18668800	2.42383800	0.65345900
C	1.21375700	3.75659600	1.05962100
H	2.16287300	4.26539400	1.18625900
C	-0.00039700	4.41146800	1.27420300
H	-0.00048300	5.44941900	1.59106700
C	-1.21444000	3.75643200	1.05949700
H	-2.16363900	4.26510300	1.18603200
C	-1.18715100	2.42367300	0.65335200
C	-0.00017300	1.69996200	0.48510300
O	-2.40499800	1.80544300	0.37254600
C	3.51409100	-0.63371000	1.06324300
C	3.15178200	-0.07070500	2.45737800
H	2.08057100	-0.07842000	2.65631800
H	3.50069800	0.95827100	2.56447000
H	3.64921900	-0.67931500	3.22160800
C	5.02106500	-0.38581100	0.85430100
H	5.55988000	-0.84872100	1.68945100
H	5.26737100	0.67820000	0.85904300
H	5.40578100	-0.83676900	-0.06285200
C	3.24261500	-2.15180000	0.99915100
H	3.52550900	-2.57743300	0.03155200
H	2.19328500	-2.39158400	1.18154000
H	3.84758500	-2.65518800	1.76216100
C	3.15348900	0.41500600	-1.90169500
C	4.40474800	1.32137600	-1.86129500

H	5.25006200	0.86718400	-1.34834400
H	4.18450800	2.28144000	-1.38855600
H	4.71930600	1.51927900	-2.89173500
C	3.49631400	-0.98015400	-2.45909900
H	3.85471800	-0.87612300	-3.48927800
H	2.61745300	-1.63390700	-2.48261500
H	4.28522500	-1.47895600	-1.89061500
C	2.13135600	1.09114400	-2.84244600
H	2.63252000	1.31903500	-3.78945000
H	1.75015600	2.03132000	-2.43379600
H	1.28425400	0.43966800	-3.06324900
C	-3.51432300	-0.63423900	1.06247200
C	-3.15253000	-0.07106700	2.45668800
H	-3.64936100	-0.68023700	3.22085900
H	-3.50238800	0.95758000	2.56384100
H	-2.08130400	-0.07776600	2.65560700
C	-3.24247700	-2.15226700	0.99840900
H	-2.19310500	-2.39183600	1.18076800
H	-3.52528100	-2.57792300	0.03078900
H	-3.84734500	-2.65580100	1.76139800
C	-5.02132800	-0.38681500	0.85317700
H	-5.40570800	-0.83801500	-0.06399800
H	-5.26798400	0.67711500	0.85773800
H	-5.56016400	-0.84979500	1.68827600
C	-3.15307300	0.41485200	-1.90230300
C	-3.49523000	-0.98033500	-2.46006800
H	-3.85356500	-0.87622400	-3.49026200
H	-4.28402100	-1.47956200	-1.89177900
H	-2.61609200	-1.63371500	-2.48368900
C	-4.40468300	1.32075200	-1.86205100
H	-4.18497400	2.28074800	-1.38892400
H	-5.25000600	0.86606200	-1.34955700
H	-4.71895700	1.51888200	-2.89253200
C	-2.13091400	1.09156900	-2.84260500
H	-1.28341000	0.44053500	-3.06316200
H	-1.75033300	2.03189500	-2.43372300
H	-2.63183700	1.31930100	-3.78977300
N	0.00034600	-2.22266700	-0.91166600
C	0.00090400	-3.27418800	-1.39753500
C	0.00218300	-4.59482600	-2.01549900
H	0.85561600	-5.17748800	-1.65714000
H	-0.91987500	-5.12811700	-1.76714700
H	0.07224500	-4.49833400	-3.10286700
H	0.00006600	0.35290400	-1.54590000

N	-0.00027200	-1.18374100	1.92292000
C	-0.00073000	-1.70572600	2.95658700
C	-0.00154800	-2.34306800	4.26714800
H	0.90422800	-2.94254800	4.39409000
H	-0.03364200	-1.57928200	5.04946100
H	-0.87593400	-2.99188600	4.36906100

Optimized Cartesian coordinates for Int5.

Ir	-0.00410000	-0.33302100	-0.35367100
P	2.24176900	0.06657500	-0.01625600
P	-2.24727400	0.06797000	0.00952600
O	2.39402600	1.75025500	-0.13816000
C	1.18760900	2.44699200	-0.09782400
C	1.22032800	3.83835200	-0.01671100
H	2.17451600	4.35768200	-0.00036200
C	0.00844000	4.53741400	0.04911000
H	0.01168000	5.62261300	0.11529200
C	-1.20643700	3.84153700	0.05279800
H	-2.15681800	4.36333200	0.12317000
C	-1.18209500	2.44944000	-0.02857800
C	-0.00021600	1.69978300	-0.13011200
O	-2.39014400	1.75672900	0.00383600
C	3.03257500	-0.17743800	1.74541100
C	2.19762700	0.72988200	2.67317500
H	1.12779800	0.54602200	2.53625400
H	2.38872100	1.78825000	2.47702300
H	2.46006500	0.52013500	3.71914100
C	4.51183300	0.21263100	1.89612300
H	4.78778800	0.19721000	2.96068700
H	4.70284500	1.22287200	1.52152700
H	5.18328800	-0.48361600	1.38466600
C	2.82106100	-1.63886000	2.18017800
H	3.43785300	-2.34106700	1.61009200
H	1.77247000	-1.92682000	2.05272900
H	3.08741000	-1.75200100	3.24027100
C	3.53313600	-0.43048100	-1.35161000
C	4.78849000	0.46496800	-1.37852200
H	5.43703900	0.31880500	-0.51416100
H	4.51105000	1.52117700	-1.42398500
H	5.37919100	0.22829400	-2.27442100
C	3.92210500	-1.90953500	-1.16314400
H	4.51467300	-2.24699300	-2.02452700
H	3.03604900	-2.54947400	-1.09736800
H	4.53079600	-2.06795100	-0.26761600

C	2.83157300	-0.28370200	-2.71882600
H	3.54008500	-0.56370000	-3.51186700
H	2.50843900	0.74651600	-2.89267700
H	1.94345700	-0.91366100	-2.78617100
C	-3.12392000	-0.25120700	1.71234000
C	-2.06596000	0.12097200	2.77119600
H	-2.45835100	-0.10204800	3.77351900
H	-1.82162800	1.18725500	2.73044000
H	-1.13908700	-0.43614100	2.60934400
C	-3.45069300	-1.74740200	1.84887000
H	-2.56951700	-2.36191400	1.63236600
H	-4.25953600	-2.05970900	1.18032700
H	-3.76941300	-1.96978500	2.87648300
C	-4.37031200	0.61747800	1.97048800
H	-5.24336200	0.29315600	1.40225200
H	-4.17044000	1.66471600	1.72836800
H	-4.63945100	0.56203000	3.03500900
C	-3.45788400	-0.38057300	-1.41913700
C	-3.21831400	-1.86154700	-1.77809800
H	-3.78871400	-2.11653000	-2.68222000
H	-3.54536100	-2.53887800	-0.98225500
H	-2.15880200	-2.05148100	-1.96786400
C	-4.95428400	-0.14366500	-1.15330900
H	-5.15657400	0.88963900	-0.85621800
H	-5.35777400	-0.81235500	-0.38772100
H	-5.51724600	-0.33698700	-2.07743100
C	-3.04656600	0.49593800	-2.62163500
H	-1.98316600	0.38033600	-2.84439300
H	-3.23979400	1.55414400	-2.42470100
H	-3.63202300	0.19353900	-3.50111400
N	0.01391000	-2.31095500	-0.31486600
C	0.03285800	-3.51641400	-0.31479700
C	0.03295100	-4.52206400	0.79590700
H	0.96546200	-5.09863400	0.78843400
H	-0.07397600	-4.03713300	1.78216700
H	-0.78295800	-5.24228600	0.66718500
H	-0.03027100	0.04170400	-1.95718900

Optimized Cartesian coordinates for Int6.

Ir	0.00134500	-0.27782800	-0.43893500
P	2.24046900	0.12584300	0.00571200
P	-2.24510900	0.11898700	-0.00710100
O	2.38407700	1.80296200	-0.27989400
C	1.18144100	2.49563200	-0.32244100

C	1.20898600	3.89102200	-0.33861200
H	2.16174800	4.41316300	-0.33740900
C	-0.00512100	4.58814600	-0.34738900
H	-0.00444800	5.67558600	-0.35512000
C	-1.21947700	3.89270600	-0.31943900
H	-2.17122000	4.41653300	-0.30374200
C	-1.19344300	2.49687100	-0.30289100
C	-0.00674200	1.75138000	-0.32844900
O	-2.39388300	1.80419500	-0.23876200
C	3.06269800	0.15295000	1.78716500
C	2.13741300	1.06772700	2.61466300
H	1.09042600	0.77096400	2.49882900
H	2.22440200	2.11263600	2.30591500
H	2.40727500	0.99974900	3.67783900
C	4.48845800	0.72309400	1.86211900
H	4.77131500	0.87732000	2.91446700
H	4.55702800	1.68948500	1.35442800
H	5.23305800	0.04668600	1.43108500
C	3.02517000	-1.25714700	2.40361300
H	3.72712600	-1.94487000	1.92267900
H	2.02695500	-1.70075900	2.34177400
H	3.30535700	-1.20084400	3.46549600
C	3.58382600	-0.48652900	-1.24618800
C	4.74691700	0.50697500	-1.44250600
H	5.39835200	0.58095300	-0.57084000
H	4.36938600	1.50665300	-1.66905600
H	5.36654400	0.17337900	-2.28717900
C	4.12862800	-1.86329200	-0.81991400
H	4.74786900	-2.27890800	-1.62706100
H	3.31970000	-2.57535100	-0.62511500
H	4.75648400	-1.80414500	0.07352300
C	2.88114700	-0.64906400	-2.61014400
H	3.61567200	-1.00390700	-3.34851800
H	2.46499000	0.29899200	-2.95925800
H	2.05250800	-1.35647900	-2.55558700
C	-3.14525700	0.10528100	1.73931500
C	-2.07800400	0.62519400	2.72258700
H	-2.45957900	0.55880800	3.75132800
H	-1.82391100	1.67058900	2.52102000
H	-1.15540600	0.04456300	2.64400000
C	-3.51985800	-1.33447800	2.13449000
H	-2.65104900	-2.00111100	2.10371000
H	-4.30273600	-1.75262500	1.49218600
H	-3.90852400	-1.34595300	3.16342700

C	-4.36612400	1.03890000	1.86183100
H	-5.25542000	0.64833200	1.36558500
H	-4.14534600	2.02614600	1.44829700
H	-4.62248600	1.16638000	2.92407400
C	-3.50623700	-0.49396100	-1.33379600
C	-3.31768400	-2.01687500	-1.48131100
H	-3.95557300	-2.39081100	-2.29477700
H	-3.59369800	-2.55832000	-0.57002400
H	-2.27915200	-2.25728400	-1.71865700
C	-4.98905800	-0.18386900	-1.06798600
H	-5.15937600	0.88643200	-0.92145500
H	-5.38153400	-0.72122600	-0.20059700
H	-5.58268800	-0.49777800	-1.93855800
C	-3.11631900	0.18536700	-2.66395100
H	-2.06941600	-0.00448500	-2.90966700
H	-3.25862200	1.26825800	-2.60925000
H	-3.75466400	-0.20843700	-3.46805000
N	0.06919900	-2.29916700	-0.63808100
C	0.12373300	-3.47420700	-0.69346300
C	0.16017500	-4.80610700	-0.07255400
H	1.10035900	-5.31746200	-0.30492100
H	0.06566200	-4.69057300	1.01692500
H	-0.65716000	-5.43285900	-0.44433100
H	-0.00510700	0.02563200	-2.06013400
O	-0.26383200	-2.68056100	2.35984600
H	-0.29084600	-2.14715000	3.16429800
H	-0.19513300	-1.99852600	1.64577700

Optimized Cartesian coordinates for Int7.

Ir	0.11976600	-0.19502500	-0.60405300
P	-2.00066800	-0.95060500	-0.04253400
P	2.33874500	0.11748500	0.02028100
O	-1.74763100	-2.62909400	0.17718200
C	-0.42287900	-3.00275600	0.34503000
C	-0.13617600	-4.30801300	0.75006000
H	-0.94524100	-5.01722600	0.90100700
C	1.19951700	-4.66853300	0.96377000
H	1.44229100	-5.67941900	1.28309400
C	2.22154000	-3.72702500	0.79781600
H	3.26114400	-3.98081900	0.98568400
C	1.88394000	-2.43393600	0.39211100
C	0.56757100	-2.03589700	0.12285400
O	2.88657300	-1.48511800	0.27213000
C	-2.93678400	-0.68419100	1.66968100

C	-1.88976400	-1.06055400	2.73665600
H	-0.94696500	-0.53204000	2.56611000
H	-1.67649500	-2.13254100	2.73061100
H	-2.26588600	-0.79037800	3.73351300
C	-4.18362100	-1.55312000	1.89800100
H	-4.51058500	-1.46883100	2.94575000
H	-3.97358900	-2.60800500	1.69955500
H	-5.02915000	-1.24118400	1.27703400
C	-3.29056100	0.80265100	1.84731200
H	-4.10125100	1.12332700	1.18656500
H	-2.42665400	1.44571500	1.65518400
H	-3.62342100	0.98292700	2.87965000
C	-3.36065000	-1.06725800	-1.42089200
C	-4.22834400	-2.33985900	-1.33327500
H	-4.88962500	-2.34989300	-0.46617100
H	-3.60266500	-3.23399100	-1.29048800
H	-4.86131100	-2.40480100	-2.22998000
C	-4.25963700	0.18447300	-1.40591700
H	-4.89186600	0.19424900	-2.30489200
H	-3.66948600	1.10734700	-1.40730900
H	-4.92786900	0.20883400	-0.54056100
C	-2.62503400	-1.11215000	-2.77628800
H	-3.37024800	-1.17565300	-3.58371300
H	-1.96305900	-1.97835800	-2.84137400
H	-2.00239600	-0.22977800	-2.93022900
C	3.04823500	0.79566400	1.73132600
C	2.02414800	0.31589000	2.77751200
H	2.27197400	0.73694800	3.76219900
H	2.02382700	-0.77516100	2.86421500
H	1.00998900	0.61831500	2.50392500
C	3.06504600	2.33371900	1.72347700
H	2.08814700	2.74461200	1.44632100
H	3.81763600	2.73732200	1.03724400
H	3.31092700	2.70997300	2.72745900
C	4.42165400	0.23739600	2.15320700
H	5.25167100	0.68915800	1.60849100
H	4.46302400	-0.84513000	2.00977600
H	4.58942800	0.44489300	3.22075800
C	3.57398600	0.64121300	-1.37157200
C	3.10181800	1.99945400	-1.92618900
H	3.72821600	2.28912300	-2.78210400
H	3.16982200	2.79961300	-1.18158700
H	2.06567900	1.93804500	-2.26468100
C	5.05604700	0.74016900	-0.97315000

H	5.41747100	-0.18959100	-0.52549100
H	5.25080300	1.56070500	-0.27737900
H	5.65848600	0.93095600	-1.87308900
C	3.45838500	-0.41838800	-2.48842700
H	2.42152500	-0.54082900	-2.80872200
H	3.81848900	-1.39177500	-2.14384600
H	4.07156800	-0.10550100	-3.34630300
N	-0.37300200	1.54761000	-1.57712600
C	-0.68107900	2.52387100	-2.13808500
C	-1.08076900	3.80663400	-2.70143200
H	-1.84473400	3.67308800	-3.47565800
H	-1.48574000	4.45610400	-1.91706500
H	-0.21983700	4.30679500	-3.15844700
H	0.34211400	-0.93578600	-2.06540100
O	-0.40483500	2.86291600	1.29976400
H	-0.29242800	2.55697000	2.20862100
H	-0.28515400	2.02845300	0.77479400
C	-2.08128200	4.88089500	1.49684600
O	-1.98367400	4.83844300	2.66202400
O	-2.25324700	5.02554900	0.34765900

Optimized Cartesian coordinates for TS4.

Ir	0.03069700	-0.15434000	0.44585500
P	2.31332800	-0.28967500	0.07837200
P	-2.22505700	-0.57130700	0.05269800
O	2.53566700	-1.86897300	-0.48733200
C	1.36891100	-2.54571400	-0.82600300
C	1.48011800	-3.79593200	-1.43344500
H	2.46322400	-4.21383300	-1.63049300
C	0.31131500	-4.48468400	-1.77632700
H	0.37579600	-5.45874700	-2.25457900
C	-0.93976300	-3.91744700	-1.51212800
H	-1.86131900	-4.43077500	-1.77109100
C	-0.99502600	-2.66409200	-0.90254300
C	0.14247300	-1.92770700	-0.53619200
O	-2.24310000	-2.11040700	-0.64571100
C	3.20681800	0.62710600	-1.37964000
C	2.42053800	0.20360200	-2.63969700
H	1.34327700	0.31637100	-2.48998000
H	2.61252100	-0.84242600	-2.89385100
H	2.73138000	0.82665900	-3.48886100
C	4.68068300	0.24595900	-1.60219400
H	5.01614800	0.65365100	-2.56631600
H	4.81802100	-0.83859000	-1.63425800

H	5.34053100	0.66294900	-0.83603000
C	3.08578200	2.15235800	-1.19819100
H	3.67770800	2.51929700	-0.35469100
H	2.04668100	2.45840100	-1.05648700
H	3.46441000	2.65448100	-2.09942100
C	3.53002200	-0.35167600	1.58396600
C	4.78326700	-1.21541700	1.32865100
H	5.48062900	-0.76641200	0.62113100
H	4.50550900	-2.20319100	0.95350700
H	5.32194700	-1.34963100	2.27687000
C	3.93834900	1.07591400	1.99448300
H	4.46644900	1.04459300	2.95717700
H	3.06442200	1.72445500	2.11883300
H	4.61069800	1.54274700	1.26953200
C	2.77175800	-0.99503900	2.76315200
H	3.45043800	-1.05411500	3.62647300
H	2.43354300	-2.00523000	2.51818300
H	1.88297100	-0.42613900	3.03678600
C	-3.34000200	0.28320100	-1.27362000
C	-2.48633400	0.35063200	-2.55848400
H	-3.08809500	0.80766900	-3.35605400
H	-2.18772800	-0.64819600	-2.89096500
H	-1.59755600	0.95971400	-2.40861700
C	-3.67300600	1.71363200	-0.81261900
H	-2.76544000	2.28973100	-0.61213900
H	-4.30351700	1.72421500	0.08397700
H	-4.22684000	2.23653800	-1.60409400
C	-4.62411600	-0.49535700	-1.63639900
H	-5.41221000	-0.40297900	-0.88996200
H	-4.41271000	-1.55694800	-1.79337700
H	-5.02546300	-0.09348100	-2.57654900
C	-3.27363400	-0.90069700	1.65123200
C	-2.99222900	0.25168900	2.63609700
H	-3.52626800	0.06520700	3.57824300
H	-3.33435800	1.21830900	2.24901500
H	-1.92397700	0.32295100	2.84963900
C	-4.79531800	-1.04359300	1.47847800
H	-5.05786400	-1.83885100	0.77617300
H	-5.27028400	-0.11463600	1.15116000
H	-5.23549700	-1.30523300	2.45092400
C	-2.74572100	-2.21867300	2.25683800
H	-1.66030500	-2.18549400	2.38181700
H	-2.99665900	-3.07336900	1.62266500
H	-3.21139900	-2.37024800	3.24076900

N	-0.07062200	1.63185900	1.49526600
C	-0.14727500	2.67907800	1.99305700
C	-0.26272500	4.03158200	2.52143100
H	0.68754400	4.35338200	2.96008600
H	-0.53343600	4.70439500	1.70062300
H	-1.03339900	4.07758600	3.29825000
H	0.03265400	-1.06319700	1.86775500
O	-0.19756000	2.45708900	-1.46951000
H	0.20132000	2.28462900	-2.33473100
H	-0.10469000	1.38753800	-0.85887800
C	-0.58780200	4.35722000	-1.53083000
O	-0.20033300	4.69998700	-2.60865900
O	-1.09400800	4.60811100	-0.47458500

Optimized Cartesian coordinates for Int8.

Ir	-0.31967400	0.02522600	0.21336700
P	-2.49922300	-0.73819400	-0.00629000
P	1.51740400	1.46893700	0.12775500
O	-3.35704200	0.62021600	-0.51576200
C	-2.57392700	1.73234100	-0.83161200
C	-3.19743500	2.84041700	-1.40629200
H	-4.26874400	2.82984800	-1.58213800
C	-2.41041500	3.94231000	-1.75335100
H	-2.87516500	4.81638300	-2.20186600
C	-1.02939300	3.92648900	-1.53605400
H	-0.40310100	4.76964300	-1.81048000
C	-0.45379800	2.79372300	-0.95820300
C	-1.19986200	1.67215000	-0.57317600
O	0.92190000	2.77531600	-0.76472200
C	-2.82664900	-1.96080700	-1.45014700
C	-2.52096800	-1.18276900	-2.74925200
H	-1.52521200	-0.73511800	-2.71970300
H	-3.25512600	-0.39106200	-2.92174300
H	-2.56333600	-1.88146200	-3.59459500
C	-4.25795500	-2.51643200	-1.56077000
H	-4.33917800	-3.09068400	-2.49297900
H	-5.00683000	-1.72032200	-1.59948000
H	-4.51022600	-3.19830500	-0.74377000
C	-1.82755500	-3.12802900	-1.31542900
H	-2.00905600	-3.72867400	-0.41799500
H	-0.79925600	-2.76213000	-1.28255400
H	-1.93041700	-3.79411500	-2.18191800
C	-3.56155800	-1.18547700	1.52156900
C	-5.08115600	-1.13309200	1.25456600

H	-5.43759400	-1.95223200	0.63123000
H	-5.36337100	-0.18861700	0.78191500
H	-5.60952100	-1.20028500	2.21432900
C	-3.14161800	-2.57441200	2.03881300
H	-3.64250700	-2.77624500	2.99437600
H	-2.06184500	-2.62600100	2.21165200
H	-3.41866400	-3.37763400	1.34911600
C	-3.25794700	-0.13488900	2.61102100
H	-3.86363400	-0.36547700	3.49743900
H	-3.51743800	0.87319800	2.27397100
H	-2.20264700	-0.12852000	2.88449800
C	3.09566800	1.03364400	-0.85287000
C	2.70087400	0.05383200	-1.97873300
H	3.60808900	-0.21107500	-2.53209600
H	1.96962200	0.49513800	-2.66289200
H	2.27902300	-0.86880400	-1.57964400
C	4.11680100	0.32446100	0.06244600
H	3.68384600	-0.52527700	0.59690300
H	4.56861400	1.00328000	0.79177300
H	4.91349800	-0.10502500	-0.55386800
C	3.72847200	2.27982600	-1.50844800
H	4.10139600	3.00337400	-0.78191000
H	3.01816300	2.79016000	-2.16367600
H	4.58044900	1.94932600	-2.11458300
C	1.95952600	2.37304000	1.75950700
C	2.30170400	1.32714500	2.83960100
H	2.45745700	1.83894900	3.79864900
H	3.21185400	0.76827700	2.60974800
H	1.47918500	0.61690700	2.96054300
C	3.10265600	3.39577900	1.61726100
H	2.89053300	4.12327300	0.82829700
H	4.06682300	2.92710000	1.41060800
H	3.20324900	3.94866300	2.56063100
C	0.69569600	3.14420200	2.20078500
H	-0.16840100	2.48093500	2.27920300
H	0.45416000	3.95175800	1.50470100
H	0.88495700	3.59007900	3.18605400
N	0.68146700	-1.71109800	0.90787800
C	1.29849700	-2.64568900	1.20673300
C	2.11983200	-3.78702000	1.56574300
H	1.76388600	-4.67733500	1.04010600
H	3.16834400	-3.57809900	1.22962400
H	2.07665500	-3.95496000	2.64681200
H	-0.60191200	0.48587200	1.79422000

O	3.39208900	-3.46439700	-1.27970600
H	3.42169500	-3.22485000	-2.21646600
H	0.01191800	-0.45337600	-1.34286600
C	4.59225800	-2.87124200	-0.77341500
O	5.29166100	-2.28696300	-1.62377900
O	4.73904100	-3.01784300	0.46305000

Optimized Cartesian coordinates for CO₂.

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16916700
O	0.00000000	0.00000000	-1.16916700

Optimized Cartesian coordinates for HCOO⁻.

C	0.00000000	0.31162100	0.00000300
H	0.00000000	1.46433000	0.00001900
O	1.14113200	-0.20837800	-0.00005800
O	-1.14113200	-0.20837800	0.00005300

Optimized Cartesian coordinates for H₂O.

O	0.00000000	0.11918900	0.00000000
H	0.75938100	-0.47675800	0.00000000
H	-0.75938100	-0.47675800	0.00000000

Optimized Cartesian coordinates for CNCH₃.

N	0.00000000	0.00000000	1.44024300
C	0.00000000	0.00000000	0.27988600
C	0.00000000	0.00000000	-1.18053500
H	0.00000000	1.02589800	-1.55926900
H	0.88845400	-0.51294900	-1.55926900
H	-0.88845400	-0.51294900	-1.55926900

Optimized Cartesian coordinates for HCO₃⁻.

O	-1.23887900	-0.53652600	-0.00008000
C	-0.15830700	0.07157700	-0.00001200
O	1.00978800	-0.79348600	0.00002300
O	0.13363100	1.29246800	0.00005700
H	1.71352700	-0.12911300	0.00007500